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THE UNIVERSITY OF ALBERTA

APPLICATION OF QUASILINEARIZATION AND LINEAR
PROGRAMMING TO CONTROL AND ESTIMATION PROBLEMS

by



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A THESIS
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The undersigned certify that they have read, and
recommend to the Faculty of Graduate Studies for acceptance,
a thesis entitled APPLICATION OF QUASILINEARIZATION AND
LINEAR PROGRAMMING TO OPTIMAL CONTROL OF AN EVAPORATOR
submitted by RONALD E. NIEMAN, B.Sc., M.Sc., in partial
fulfilment of the requirements for the degree of Doctor
of Philosophy.



ABSTRACT

This thesis describes the development and application of quasilinearization and linear programming techniques to the solution of problems associated with the adjustment of process data, estimation of parameters in process models, and the design of optimal state driving control systems. Experimental data from a computer controlled pilot plant evaporator are used to demonstrate the practicality and potential industrial importance of each application.

A data analysis program, which is independent of the application, performs the data acquisition, filtering, statistical analysis and data adjustment. The program was used routinely to produce a consistent set of evaporator data for later analysis.

An extensive literature review and comparison of process identification and parameter estimation techniques and their applications is presented as a guideline for choosing a suitable method for a specific application.

The literature review and previous work showed that quasilinearization was a powerful method for handling the parameter estimation problem. Quasilinearization was combined with linear programming to produce a generalized parameter estimation computer program which had adequate flexibility to be able to incorporate a priori knowledge and

constraints of the process which is being identified.

A convenient constrained parameter perturbation technique was developed which increased the region of convergence of the parameter estimation algorithm.

Linear programming techniques were used alone to solve the dynamic optimization associated with the calculation of the optimal control strategy. A standard state-space model and a linear performance index was employed. Quasilinearization and linear programming were used for the identification of process models. Experimental and simulated results from a pilot plant evaporator indicate improved performance over conventional feedback control for set point changes.

Optimal control proved to be sensitive to model accuracy. A fifth order theoretical linear model which agreed reasonably well with the open loop process response was not satisfactory for determining optimal control policies. Fitted models performed better. Policies based on a reduced model were satisfactory if the switch times were tuned experimentally but constraints could not be incorporated.

A new approach for adding optimal state driving control policies to conventional multiloop or optimal multivariable feedback control systems is demonstrated to be simple and convenient. The simpler open-loop process model can be used for the calculations and "automatic" transfer to regulatory control facilitates implementation.

For more difficult applications such as plant startup, suboptimal control policies are calculated using nonlinear process models by formulating the problem as one of identifying parameters in an assumed control law. This approach gives the designer more flexibility by permitting, for example, a reduction in the number of switching times to simplify implementation.

The listings of the FORTRAN programs used in this work and some user oriented documentation were reproduced and bound separately from the thesis.

Use of all the developed procedures and programs on realistic engineering problems indicated that they are practical and should be of use in industrial applications.

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TABLE OF CONTENTS

	<u>Page</u>
CHAPTER ONE INTRODUCTION	1
1. General	2
2. Scope of This Work	3
3. Status of Work	5
4. Thesis Format	6
CHAPTER TWO A REVIEW OF PROCESS IDENTIFICATION AND PARAMETER ESTIMATION TECHNIQUES	7
1. Introduction	8
2. Parameters in Ordinary Differential Equations	31
3. Parameters in an Analytical Solution	48
4. Parameters in a Discrete Model	53
5. Coefficients in a Functional Series Expansion	62
6. Impulse Response	69
7. Frequency Response	80
8. Conclusions	91
CHAPTER THREE PARAMETER ESTIMATION USING QUASI- LINEARIZATION AND LINEAR PROGRAMMING	92
1. Introduction	93
2. Formulation and Theory of Quasi- linearization	96
3. Computational Aspects	99

	Page
CHAPTER THREE (Cont'd)	
4. Linear Estimation	102
5. Prediction of the Reliability of Parameters and Accuracy of the Model	108
6. Promotion of Convergence	111
7. Results	112
8. Conclusions	132
CHAPTER FOUR COMPUTER CONTROL USING OPTIMAL STATE DRIVING TECHNIQUES 134	
1. Introduction	135
2. Literature Review	137
3. Description of Equipment	139
4. Process Modelling and Identification	139
5. Formulation of the Optimal Control Problem	143
6. Discussion of Results	149
7. Conclusions	178
CHAPTER FIVE OPTIMAL STATE DRIVING CONTROL TECHNIQUES COMBINED WITH CONVENTIONAL REGULATORY SYSTEMS: AN EXPERIMENTAL EVALUATION 180	
1. Introduction	182
2. Literature Review	184
3. Formulation of the Optimal Control Problem	186
4. Comparison of Criteria - A Numerical Example	194

	Page
CHAPTER FIVE (Cont'd)	
5. Interfacing an Optimal Control System to a Conventional Closed Loop Control Scheme	200
6. Implementation on a Double Effect Evaporator System	203
7. Conclusions	240
CHAPTER SIX SUBOPTIMAL CONTROL OF NONLINEAR SYSTEMS	
1. Introduction	243
2. Development	244
3. Computational Aspects	248
4. A Nonlinear Numerical Example	249
5. Application to a Double Effect Evaporator	251
6. Conclusions	257
CHAPTER SEVEN DISCUSSION AND CONCLUSIONS	
1. General	259
2. Industrial Use	259
3. Application to Other Problems	261
4. Future Work	266
5. Conclusions	269

NOMENCLATURE

Chapter Three	272
Chapter Four	274
Chapter Five	276
Chapter Six	277

BIBLIOGRAPHY

Chapter One	278
Chapter Two	279
Chapter Three	319
Chapter Four	322
Chapter Five	324
Chapter Six	326
Chapter Seven	327

APPENDICES

General	328
A Equipment Description	328
B Model Documentation	331
C Run Documentation	342
Chapter Three	
1. Derivation and Performance Evaluation of Nonlinear Gain Expression	348

LIST OF TABLES

	<u>Page</u>	
CHAPTER TWO		
Table 1	Classification of Current Methods of Identification	13
Table 2	Comparison of Statistical Estimation Methods	25
CHAPTER THREE		
Table 1	Constrained Parameter Stepping Procedure	120
Table 2	Seven Constant Reaction Model Identification	126
Table 3	Comparison of Least Squares and Chebyshev Solutions to the Four Constant Reaction Model Identification	129
Table 4	Van der Pol Problem Results	133
CHAPTER FOUR		
Table 1	Parameters in Second Order Fitted Models	160
CHAPTER FIVE		
Table 1	Various Model Parameters	206
CHAPTER SIX		
Table 1	Time Optimal Switch Times	250

LIST OF FIGURES

	<u>Page</u>	
CHAPTER TWO		
1	Model Reference Approach to Parameter Estimation	42
2	Identification of the Impulse Response Via Correlation Techniques	76
CHAPTER THREE		
1	Flow Diagram of the Parameter Estimation Algorithm	98
2	Product Concentration Response to 20% Steam Step	114
3	Product Concentration Response to Steam Disturbances	116
4	Convergence of Nonlinear Kinetics Example Using Constrained Parameter Technique (Data Set One)	121
5	Final Solution of Nonlinear Kinetics Example (Data Set One)	122
6	Solution to Chemcell Problem (80°C) for Data Set One	127
CHAPTER FOUR		
1	Schematic Diagram of Double Effect Evaporator	140
2a	Simulated Responses of Concentrations and Liquid Levels Under Optimal, Closed-Loop and Open-Loop Control	150
2b	Simulated Responses of Flow Rates and Temperature Under Optimal, Closed-Loop and Open-Loop Control	151

CHAPTER FOUR (Cont'd)

3a	Responses of Concentrations and Liquid Levels for Optimal Control Based on First Order Models	153
3b	Responses of Flow Rates and Temperature for Optimal Control Based on a First Order Model	154
4	Experimental Response for Real Time Switching Based on First Order Model	157
5	Experimental Response for Real Time Switching Based on First Order Model	158
6a	Responses of Concentrations and Liquid Levels for Optimal Control Based on Second Order Models	162
6b	Responses of Flow Rates and Temperature for Optimal Control Based on Second Order Models	163
7	Simulated Evaporator Response for Real Time Switching Based on Second Order Model	166
8	Experimental Response for Real Time Switching Based on Second Order Model	168
9	Experimental Response for Real Time Switching Based on Second Order Model	169
10a	Responses of Concentrations and Liquid Levels for Control Based on Model 5L1 (IP-W1, W2, C2)	171
10b	Responses of Temperature and Flow Rates for Control Based on Model 5L1 (IP-W1, W2, C2)	172
11a	Response of Concentration and Liquid Levels for Control Based on Model 5L1 (IP-C2)	176
11b	Response of Temperature and Flow Rates for Control Based on Model 5L1 (IP-C2)	177

CHAPTER FIVE

1	Schematic Diagram of Gas Absorber System	195
2	Response of x_6 for Different Criteria	198
3	Response of x_3 for Different Criteria	199
4	Addition of Open-Loop Optimal Control Policy to Existing Regulatory Control Scheme	202
5	Schematic Diagram of Double Effect Evaporator	204
6a	Response of Concentration and Liquid Levels for Time Optimal Control Based on Model 5L	209
6b	Response of Flow Rates and Temperature for Time Optimal Control Based on Model 5L	210
7a	Response of Concentration and Liquid Levels for Time Optimal Control Based on Model 5LF	212
7b	Response of Flow Rates and Temperature for Time Optimal Control Based on Model 5LF	213
8a	Response of Concentration and Liquid Levels with Fast Liquid Level Recovery for $t > t_f$	216
8b	Response of Flow Rates and Temperature with Fast Liquid Level Recovery for $t > t_f$	217
9a	Concentration and Liquid Level Response of Model 5NL to Control Policies Derived from Model 5L and Model 5LD	219
9b	Flow Rates and Temperature Response of Model 5NL to Control Policies Derived from Model 5L and 5LD	220
10a	Concentration and Liquid Level Response to Control Based on Model 5LF, SAE Criterion	223

CHAPTER FIVE (Cont'd)

10b	Flow Rate and Temperature Response to Control Based on Model 5LF, SAE Criterion	224
11	Simulated Response to Control Based on Second Order Model 1	226
12	Experimental Response to Control Based on Second Order Model 1	227
13	Simulated Response to Control Based on Second Order Model 2	229
14	Simulated Response to Control Based on Model 2 with (-20%) Feed Disturbance	230
15	Experimental Response to Control Based on Model 3 with (-10%) Feed Disturbance	231
16	Experimental Response to Control Based on Model 3 with (+25%) Feed Disturbance	232
17	Simulated Response to Control Based on Model 2 with (+10%) Feed Disturbance	234
18a	Experimental Response to Control Based on Model 5LF, SAE Criterion	235
18b	Experimental Response to Control Based on Model 5LF, SAE Criterion	236
19a	Experimental Response to Control Based on Model 5LF, SAE Criterion	238
19b	Experimental Response to Control Based on Model 5LF, SAE Criterion	239

CHAPTER SIX

1	Response of Model 5NL to Suboptimal Control Strategies	253
2	Assumed Control Law for Steam	255

CHAPTER ONE

INTRODUCTION

The motivation, scope and status of the work presented is outlined so as to maintain continuity throughout the thesis. The thesis format which consists of several relatively independent chapters is revealed for clarity.

1. GENERAL

The Data Acquisition, Control and Simulation Center in the Department of Chemical and Petroleum Engineering at the University of Alberta houses an IBM 1800 process control computer which has the capability of data acquisition, data reduction, direct digital control (DDC) and programmed control. Since the spring of 1968 the control computer has been interfaced to several pilot-plant sized processes and a series of computer control studies have been implemented. Studies involving feed forward and multiloop feedback control schemes on an evaporator [1,2] and a distillation column [3,4,5] were implemented and demonstrated several advantages over conventional single variable feedback control schemes. More recently multivariable computer control has led to investigations of optimal regulatory control designed using dynamic programming [6]. Development of an on-line program [7] for efficient automatic startup is near completion.

This work at the University of Alberta, and elsewhere, has been paralleled by growing industrial acceptance of computer control [8] and installation of real-time digital computers which have the capability of implementing multivariable control systems. Also a great deal of theoretical work in the area of optimal multivariable control theory has been completed in recent years and great potential for improved control is evident. Design of optimal multivariable control systems employs the

state representation and modern dynamic optimization techniques.

2. SCOPE OF THIS WORK

The previous work indicated a need for a general parameter estimation procedure for the identification of process models and an optimal multivariable control system to augment feedback control for setpoint changes or state driving applications. This work is concerned with the application of quasilinearization and linear programming techniques to the design of a servomechanism control system. Experimental testing and evaluation is performed on a pilot plant evaporator equipped with conventional instrumentation. Emphasis is placed on the practical details of implementation and operation as well as the theory.

The overall design of the optimal state driving control system involves several steps:

1. computer acquisition and adjustment of data for use in characterizing the process and defining the control problem.
2. modelling and identification of the process.
3. dynamic optimization based on a process model.
4. implementation of an optimal state driving control policy.

The following subsections outline the work performed in each of these areas:

2.1 Data Acquisition and Adjustment

Before identification, simulation or control analysis is performed, it is desirable to have a consistent set of data which satisfies physical constraints such as the process material and energy balances. A generalized program is described in reference [9] which performs on-line data acquisition, calculation of errors of closure in the steady state mass and energy balances, statistical testing for consistency of the data and adjustment of the data to provide a consistent set of data. This program is executed as a standard step in the data processing procedure for each experimental run performed on the evaporator. Linear programming was used as a method for the adjustment of the raw process data.

2.2 Process Parameter Estimation

A general parameter estimation algorithm was developed since the need existed, not only for the reduction of process data in control applications, but also in other areas such as in the analysis of kinetic data. Quasilinearization combined with linear programming was chosen for two main reasons:

1. Donnelly [10] had previously worked with quasilinearization as a numerical method.
2. an extensive search of the literature indicated this approach to be general and powerful.

The quasilinearization plus linear programming algorithm was used to fit parameters in control models, for use in state driving control applications.

2.3 Optimal State Driving

Often in industrial processes it is required to change operating conditions. The optimal control problem is to accomplish this transition while minimizing a performance index (eg. minimum time). A standard linear programming system was used for the dynamic optimization of the multi-variable model response because it is commonly used in industry and it enables a priori knowledge and constraints to be incorporated into the problem solution. The optimal control strategy is produced as a discrete time series which can be conveniently introduced into a DDC control scheme.

For more difficult applications such as plant startup it is advisable to work with the nonlinear model. A technique is presented in which the functional form of the control law is assumed and the parameters are optimized. This approach gives the designer a certain degree of flexibility which does not exist in true optimal control techniques. Such a design approach is applicable to conventional PID control, "suboptimal" control laws and optimal control laws for certain classes of problems.

3. STATUS OF WORK

In chapter seven a discussion of the implementation, extensions and industrial uses of these techniques indicates that this work serves as a starting point for industrial application of the techniques studied in previous chapters.

4. THESIS FORMAT

Chapters two through six are written in a format comparable to that used by most technical journals with the objective of providing a concise and complete presentation. Each chapter is relatively independent of others and can be conveniently accessed by a reader interested in only certain aspects of the thesis but this necessitated some duplication of material.

The thesis is supplemented by manuals containing detailed documentation of the computer programs and algorithms. These manuals have been bound separately for convenience since they are not necessary to this presentation of research results and are on file in the Department of Chemical and Petroleum Engineering.

CHAPTER TWO
A REVIEW OF PROCESS IDENTIFICATION AND
PARAMETER ESTIMATION TECHNIQUES

ABSTRACT

A survey of the recent literature in the area of process identification and parameter estimation techniques applicable to lumped-parameter, deterministic, dynamical systems is presented. Methods reviewed include statistical estimation techniques, direct and indirect methods based on optimal control theory, functional expansion, impulse response, frequency response and a number of other specific methods. Each method is presented in a consistent format which includes an outline of the general characteristics, calculational techniques, experimental techniques, reliability estimates and applications. The overall objective is to provide a basis for comparison of the methods and a guide to particular applications which will assist the reader in selecting the best method for his specific problem.

1. INTRODUCTION

Mathematical models which adequately characterize the dynamic performance of physical systems are essential for most modern control analysis, optimization and design methods. In some instances there is no a priori information about the system and the topology of the model must be determined from experimental tests or defined by assuming some empirical form. In other cases the functional form of the model and perhaps some of the parameters, are known from theoretical analysis or previous tests. However, in almost all cases complete specification of the model requires estimation of unknown parameters of the model, based on experimental data. Many techniques are applicable to these process identification and parameter estimation problems, but each is limited to problems with specific characteristics or by the experimental techniques or data that are required.

At the 1967 I.F.A.C. Symposium on "Process Identification in Automatic Control Systems" in Prague, sixty-five papers were presented. Godfrey and Hammond [1] summarize some of the main topics of discussion at this meeting and conclude that although there are many techniques available there seems to be no logical basis for choosing between them and that there are relatively few applications which have been presented in the literature. This paper was written with the hope of contributing to the solution of this dilemma. However, in order to keep this presentation to a reasonable size the author has:

- (1) restricted it to lump-parameter, deterministic, dynamical systems and specifically omitted distributed parameter systems [2,3,4], stochastic systems and most of the techniques that are suitable for only steady-state (algebraic) systems;
- (2) referred extensively to existing papers or texts for definitive and/or detailed discussion;
- (3) concentrated on recent literature and omitted most of the material included in previous surveys, in the bibliography of major referenced papers or which dealt with material which was judged to be adequately covered by other references quoted herein; and
- (4) relied, in many cases, on the title and the data included in the list of references to define the particular subject area and the chronological order of the various works.

The primary organization of this paper is based on the following classification of the problems to which techniques can be applied to estimate:

- (a) Parameters in ordinary differential equations;
- (b) Parameters in an analytical solution;
- (c) Parameters in a discrete model;
- (d) Coefficients in a functional series expansion;
- (e) Impulse response;
- (f) Frequency response.

A secondary division is based on the specific estimation techniques which apply to each classification of problem. Some of the divisions may appear arbitrary but the criterion used for creating a specific problem classification or division between estimation techniques was whether there was a significant amount of literature dealing with the subdivision and/or whether in the author's opinion it improved the clarity of the presentation. It will be noted that the first column of Table 1 is a list of the problem classifications plus the applicable estimation techniques. The balance of Table 1 represents a summary and a comparison of the main features of each estimation technique. (The terminology is defined in Section 1.1).

Each estimation technique is discussed further in the sections of this report bearing the same number as used in Table 1 and includes subsections dealing with:

- (a) General discussion;
- (b) Computational techniques and reliability estimates;
- (c) Experimental techniques;
- (d) Applications.

The balance of this introduction is devoted to a summary of the principal characteristics of estimation techniques, a discussion of the reliability of parameter estimates and a brief review of some of the basic statistical estimation methods which are used extensively in parameter estimation.

1.1 Principal Characteristics of Estimation Techniques

Process identification and parameter estimation techniques differ significantly with respect to the type of model to which they can be applied, the criterion selected, the calculation techniques that must be used, the test signal that is used to perturb the system, and the type and amount of experimental data that are required or can be handled. There are many excellent review articles which survey the literature and discuss these general characteristics. A paper by Cuenod and Sage [5] presented at the 1967 I.F.A.C. Symposium reviews many of the current methods and illustrates them with simplified examples. Eykhoff, in a paper presented at the same meeting [6] and in an earlier article [7], takes a different approach towards discussion of many of the same methods. Balakrishnan and Peterka [8] classify identification methods with respect to criterion of optimality, the mathematical model used, the computing technique and the input signal. Characterization of non-linear systems is considered by Harris and Lapidus [9] and Aleksandrovskii and Deich [10]. More recent review articles which are cited later in this paper and are recommended to the reader seeking a broader perspective include those by Bard and Lapidus [11], Seinfeld [12] and Young [13,14]. The proceedings of the 1970 I.F.A.C. Symposium on "Process Identification and Parameter Estimation", held in Prague, also include an excellent review article by Astrom and Eykhoff [15] and many pertinent papers.

The characteristics used in this paper as a basis for comparing identification and estimation techniques are defined in the following subsections and also comprise the column headings in Table 1.

(a) A priori structure

Following the general approach taken by Harris and Lapidus [9] and Eykhoff [16] the amount of information available about the structural configuration, or functional form, of the model can be classified as none, partial or complete

- (i) No available information - in this case, the topology or structural configuration of the "black box" process must be determined in addition to generating numeric estimates of specific parameters [5,16,17]. 'Process identification' usually refers to the experimental determination or approximation of the system topology.
'Parameter estimation' deals with generating numeric estimates of specific parameters or coefficients in the system model and usually follows any process identification procedure [9]. Some procedures consist of a series of parameter estimation problems using different assumed models [18] followed by model discrimination procedures to select the 'best' model [15].
- (ii) Partial information available - information about the structural configuration of the model plus

Table 1

Classification of Current Methods of Identification

MODEL										TEST SIGNAL				DATA	
	(a) A Priori Structure	(b) State Linearity	(c) Dimension	(d) Discrete/Continuous	(e) Parameters Constant/Varying	(f) Handle Time Delays	(g) Constraints	(h) Signal Dependent	(i) Sensitivity to Disturbances	(j) All States Accessible	(k) Data Processing	(l) Data Sets			
2.0 PARAMETERS IN ORDINARY DIFFERENTIAL EQUATIONS															
2.1 Differential Approximation	complete	both	mimo	continuous	constant	possible	no	yes	no	yes	non-sequential	multiple			
2.2 Parameter Optimization	complete	both	mimo	continuous	constant	possible	no	no	no	no	non-sequential	multiple			
2.3 Methods Based on Optimal Control	complete	both	mimo	continuous	varying	varies	no	no	no	no	sequential	varies			
2.4 Model Reference	complete	both	mimo	continuous	non-sequential	non-sequential	no	no	no	no	non-sequential	single			
2.5 Step Response	complete	linear	siso (<2 order)	continuous	constant	non-sequential	yes	yes	yes	yes	non-sequential	single			
2.6 Repeated Integration	complete	linear	siso (low order)	continuous	constant	non-sequential	no	no	no	no	non-sequential	multiple			
3.0 PARAMETERS IN AN ANALYTICAL SOLUTION															
3.1 Search Techniques	complete	both	mimo	continuous	constant	possible	no	no	no	no	non-sequential	multiple			
3.2 Prony's Method	complete	linear	siso (low order)	continuous	constant	possible	no	no	no	no	non-sequential	single			
4.0 PARAMETERS IN A DISCRETE MODEL															
4.1 Statistical Estimation	complete	both	mimo	discrete	varies	possible	no	no	no	no	non-sequential	multiple			
4.2 Kalman Filtering	complete	both	mimo	discrete	varies	possible	no	no	no	no	non-sequential	single			
5.0 COEFFICIENTS IN A FUNCTIONAL SERIES EXPANSION															
5.1 Volterra Expansion	none	both	siso	constant	constant	N/A	no	yes	yes	yes	non-sequential	single			
5.2 Wiener Theory	none	both	siso	constant	constant	N/A	no	no	no	no	non-sequential	single			
6.0 IMPULSE RESPONSE															
6.1 Direct Impulse Testing	none	linear	siso	continuous	constant	yes	no	no	no	no	non-sequential	single			
6.2 Deconvolution	none	linear	siso	continuous	constant	yes	no	no	no	no	non-sequential	single			
6.3 Correlation Techniques	none	linear	siso	continuous	constant	yes	no	no	no	no	non-sequential	both			
6.4 Method of Moments	complete	linear	siso (<2 order)	continuous	constant	yes	no	no	no	no	non-sequential	single			
7.0 FREQUENCY RESPONSE															
7.1 Frequency Response Testing	none	linear	siso	continuous	constant	no	yes	yes	yes	yes	non-sequential	single			
7.2 Pulse Testing	none	linear	siso	continuous	constant	no	no	no	no	no	non-sequential	single			
7.3 Frequency Response from Transient Response	none	linear	siso	continuous	constant	no	yes	yes	yes	yes	non-sequential	single			
7.4 Frequency Response from Spectral Analysis	none	linear	siso	continuous	constant	no	no	no	no	no	non-sequential	single			

estimates or limits on some of the parameters can frequently be used to select a suitable functional form for the model and/or simplify the identification and parameter estimation problem. A chemical reaction system in which only part of the reaction mechanism is known typifies this definition. In some applications a priori information is used only to generate the starting point and/or to constrain parameters and promote convergence of the numerical calculations associated with the selected estimation technique.

- (iii) Complete information available - by definition, the process identification step is complete and all that remains is the parameter estimation problem. A reaction system described by an assumed mechanistic, kinetic model but with unknown rate constants falls into this category.

(b) State Linearity

Although most physical problems are non-linear, a linearized model is often used to approximate the system response because of the simpler form of the model, the resulting simplification of the parameter estimation and the wider range of control theory that has been developed for linear systems. When the model is to be used to predict system behaviour about some nominal set of values, such as normal plant-operating conditions, then the linear model

is frequently adequate. It can, however, give misleading information about system stability, the global optimum and even steady-state responses.

A non-linear system can be represented in the following mathematical form:

$$\dot{\underline{x}} = \underline{f}[\underline{x}(t), \underline{u}(t), \underline{p}(t)] \quad (1)$$

$$\underline{y}(t) = \underline{h}[\underline{x}(t), \underline{u}(t)] + \underline{v}(t) \quad (2)$$

where

$\underline{x}(t)$ = state vector ($n \times 1$),

$\underline{u}(t)$ = input or control vector ($m \times 1$)

(corrupted by noise in general),

$\underline{p}(t)$ = unknown parameters vector ($p \times 1$),

$\underline{y}(t)$ = output vector ($r \times 1$),

$\underline{v}(t)$ = measurement noise ($r \times 1$).

The parameter estimation problem is to determine $\underline{p}(t)$ such that the model 'best fits' the given experimental data, $\underline{y}(t)$, according to an assumed criterion. Usually the experimental data are a series of discrete values of the output variables at various values of the independent variable for a known or measured perturbation in the input vector \underline{u} .

In some cases the order of the model, n , is unknown [19]. Also techniques are available for reducing mathematical models to their "minimal parametric representation" [15,20-22].

For the special case of linear systems equations (1) and (2) reduce to:

$$\dot{\underline{x}}(t) = \underline{A}(t) \underline{x}(t) + \underline{B}(t) \underline{u}(t) \quad (3)$$

$$\underline{y}(t) = \underline{C}(t) \underline{x}(t) + \underline{v}(t) \quad (4)$$

where the unknown parameters appear in $\underline{A}(t)$ and/or $\underline{B}(t)$.

The most important characteristic of the analysis of linear systems is the applicability of the principle of superposition. The process identification problem is again stated in a similar fashion.

Time-invariant systems are an important sub-class of linear systems and can be represented by:

$$\dot{\underline{x}}(t) = \underline{A}\underline{x}(t) + \underline{B}\underline{u}(t) \quad (5)$$

$$\underline{y}(t) = \underline{C}\underline{x}(t) + \underline{v}(t) \quad (6)$$

where the unknown parameters are constants which appear in the matrices \underline{A} and/or \underline{B} . It must be emphasized that the linearity referred to in this section is with respect to the state variables and not with respect to the parameters. Even a linear time-invariant system such as one represented by equation (5) results in a non-linear parameter estimation problem. This follows from the fact that most techniques for estimating parameters in a differential equation actually integrate the equations and then estimate the parameters in the resulting algebraic expressions $\underline{x}(t)$. For example, the solution to (5), assuming zero initial condi-

tions and a disturbance introduced at time zero, can be written [22] as:

$$\underline{x}(t) = \int_0^t \underline{\phi}(t - \xi) \underline{B}u(\xi) d\xi \quad (7)$$

where

$$\underline{\phi}(t - \xi) = \exp [\underline{A}(t - \xi)]$$

When unknown parameters occur in the A matrix the estimation problem is obviously non-linear.

(c) Dimension

Some techniques will handle Multiple Input, Multiple Output (MIMO) systems while others are restricted to Single Input, Single Output (SISO) analysis. A further restriction arises because some techniques are only practical for low-order systems. A set of SISO systems may be used to model a MIMO system, for example, a matrix of transfer functions.

(d) Discrete/Continuous

The mathematical models defined by equations (1) to (6) are continuous but can also be formulated in discrete form and most estimation techniques can be formulated to handle either case (reference section 4.0). It is important to note that for practical applications many of the mathematical operations involved in the 'continuous' formulations are approximated by numerical methods. (The most common example is integration). Thus, in many cases, even the

'continuous' techniques are implemented using numerical techniques and time series of discrete data.

(e) Parameters Constant/Varying

In some model formulations such as equations (1) to (4) the parameters are assumed to be functions of time while in others, for example equations (5) and (6), they are assumed to be time invariant or constant. It should be noted that most methods that handle time-variant systems will also handle time-invariant problems, but the calculational effort (computer time) is often significantly greater than techniques designed to deal specifically with time-invariant systems. In general, a linear model with time-varying parameters will more accurately approximate a non-linear system than a linear model with constant coefficients.

(f) Handle Time Delays

The pure time delay (transport lag) is a feature of many physical systems, particularly in the process industries, and must be incorporated into the model. In these situations the ability to estimate the time delays without significantly complicating the analysis will be an important factor in selecting the estimation technique [23].

(g) Constraints

In most systems the actual values of at least some of the parameters are constrained by physical limits or conservation laws. For example, many parameters cannot be

negative. Estimation techniques vary tremendously in their ability to include constraints.

For those methods (e.g. Kalman filtering) which generate estimates of the state vector, \underline{x} , coincident with the estimate of the parameters, then constraints on the states might also be considered.

(h) Signal Dependent

In some cases the choice of the estimation technique defines the input or forcing function that must be used to excite the system. For example, classical frequency response analysis necessitates the use of pure sinusoidal variations in the forcing variable. In some cases, it may not be practical or convenient to generate the required signal and hence techniques can be rejected on this basis. In general, the techniques with the fewest restrictions on choice of the forcing function have the most sophisticated data-processing (highest computer time) requirements. Frequently even the general methods that are 'signal independent' can be simplified by proper choice of the forcing function. The choice of test signal also influences the accuracy and/or precision of the parameter estimates and the total experimental time or amount of data required. Several papers discuss the selection of test a signal [24-30].

The broader question of experimental design to eliminate factors such as bias produced by different process operators, aliasing of some effects by others, unnecessary replicates, etc. are as important in the area of parameter estimation as in any other experimental study. Texts exist in this area [31] and many publications deal with the 'sequential' (vs. a priori) approach to experimental design [11,32,33] and techniques for relating the experiments to the assumed model [34].

(i) Sensitivity to Disturbances

In practical applications the test signals are often corrupted by noise or confounded with uncontrolled disturbances which enter the system. Some estimate of the sensitivity of the estimation methods to disturbances is given in column (i) of Table 1. Obviously the methods that are signal dependent cannot tolerate large random disturbances. In other methods the random disturbances, if they can be measured, can frequently be handled as known inputs. Some techniques are more tolerant of noise than others but, in general a decrease in the signal-to-noise ratio decreases the reliability of the parameter estimates. In extreme cases stochastic methods must be used but these are not dealt with in this paper.

(j) All States Accessible

Some methods can be used with measurements of only some of the output variables, \underline{y} ; others require measurements

for all output variables; other more restrictive methods require measurements or 'observability' of all of the state variables, \underline{x} , and some require the time derivative of the state, $\dot{\underline{x}}$. "Observers" or filters can be used to generate \underline{x} or $\dot{\underline{x}}$ [35] but only the "completely controllable and observable" part of the model can be determined from input-output measurements [15,22].

(k) Data Processing

With some estimation techniques all the data must be collected before data analysis begins and a single estimate of the parameters is produced. In computer terms this is normally an off-line, batch job. Other techniques, usually referred to as 'sequential', can be executed in 'real-time' and use the data obtained at each time interval to produce an updated estimate of the parameters.

(l) Data Sets

Some estimation techniques will accept only a single set of data (replicates can be averaged and used). The more powerful techniques will handle multiple data sets even if they are taken under different (known) conditions. Multiple data sets are represented in this paper by subscripted vectors, \underline{y}_N .

1.2 Reliability Estimates

Reliability estimates of the parameters should be an integral part of every parameter estimation problem. They not only indicate the degree of confidence that should be

placed on the results but can also play an important role in maximizing the information gained from subsequent experiments [11]. For this reason a discussion of reliability estimates is included in most of the following sections. However, the following general points deserve emphasis.

Rosenbrock and Storey [36] derive an expression for the covariance matrix of parameters determined using the least squares technique. Heineken et al. [37] apply this technique to the estimation of confidence limits for enzymatic reactions. The Cramer-Rao inequality [38] is often used to determine a limit on the accuracy of the parameter estimates.

A problem related to the estimation of parameter reliability is the definition of an 'adequate' model. The suitability of a particular model form is usually strongly dependent on the application or end-use of the model. For example, regulatory control systems demand much less of a model than a servomechanism as will be demonstrated in Chapters 4 and 5. Gupta [39] discusses a quadratic criterion useful for model comparison and discrimination.

Frequently it is the reliability of the output responses predicted from the model that is of interest rather than the reliability of the parameters themselves. For example, a very low reliability for a parameter that has a negligible effect on the model output, at least for conditions of current interest, need not be of concern.

Since a function of a random variate is itself a random variate, a first-order Taylor's series expansion of the model output in terms of the parameters can be used along with reliability estimates for the parameters to furnish an estimate of the model accuracy.

Balakirev and Golubev [40] compare the accuracy of several methods from fourteen previous papers.

1.3 Statistical Estimation Methods

In many instances the estimation of parameters in a dynamic model can be reduced to the simpler problem of estimating parameters in an algebraic model (cf. section 2.1 and 4.1). Since the latter estimation problem has received considerable attention in textbooks and other published references, only a brief introduction to statistical estimation methods will be presented here. A more extensive treatment can be found in textbooks on mathematical statistics, the text by Deutsch [41], and recent review articles [6,14,15,42,43].

For purposes of discussion, we consider the algebraic model in equation (8) which relates a scalar output y to the parameters $\underline{k} = [k_1, \dots, k_p]^T$ and inputs $\underline{x} = [x_1, \dots, x_n]^T$

$$y = f(\underline{x}, \underline{k}) + \epsilon \quad (8)$$

The scalar ϵ is referred to as the residual or error and by definition is the difference between the observed output

y and the model output $f(\underline{x}, \underline{k})$. The observed values of y are denoted as y_1, y_2, \dots, y_N and the corresponding observations of \underline{x} as $\underline{x}_1, \underline{x}_2, \dots, \underline{x}_N$. The classical parameter estimation problem is to determine an estimate \underline{k} such that $f(\underline{x}, \underline{k})$ gives the 'best fit' to the observed values y_i as defined by some criterion of optimality (i.e., performance index).

Statistical estimation methods are usually classified according to the performance index that is selected and the a priori knowledge about the residuals that is utilized. These features are summarized in Table 2 for the least-squares, maximum-likelihood and Bayesian estimation techniques.

(a) Least_Squares [6,14,41]

In this popular approach the objective is to determine the parameter estimate \underline{k} which minimizes S , the sum of the squared residuals for the N observations:

$$S = \underline{\epsilon}^T \underline{\epsilon} = \sum_{i=1}^N \epsilon_i^2 \quad (9)$$

where

$$\epsilon_i = y_i - f(\underline{x}_i, \underline{k}) \quad (10)$$

If the model equations are linear in the parameters \underline{k} , but not necessarily in the inputs \underline{x} , the minimization results in an analytical expression for $\hat{\underline{k}}$ and the approach is referred to as linear least squares or multiple linear regression.

TABLE 2

COMPARISON OF STATISTICAL ESTIMATION METHODS

Method	Performance Index	A priori knowledge	Properties of linear estimates	Comments
1. Least squares	$\min_{\underline{k}} \underline{\epsilon}^T \underline{W} \underline{\epsilon}$	None	Unbiased	
2. Weighted least squares	$\min_{\underline{k}} \underline{\epsilon}^T \underline{W} \underline{\epsilon}$	None (or $E[\underline{\epsilon} \underline{\epsilon}^T]$)	Unbiased, efficient	Choice of $\underline{W} = E[\underline{\epsilon} \underline{\epsilon}^T]^{-1}$ gives minimal variance estimate
3. Maximum likelihood	$\max_{\underline{k}} p(\underline{y} \underline{k})$	Form of $p(\underline{\epsilon})$	Unbiased, efficient sufficient, asymptotically normal if $\{\epsilon_i\}$ are independent	Parameters of $p(\underline{\epsilon})$ can be calculated, if unknown
4. Bayesian estimation	Various performance indices are used (see text)	Form of $p\left(\frac{\underline{\epsilon}}{\underline{k}}\right)$, $p\left(\frac{\underline{k}}{\underline{k}}\right)$	Minimum risk, same as maximum likelihood if $p\left(\frac{\underline{k}}{\underline{k}}\right) = \text{uniform distribution}$	Parameters of $p(\underline{\epsilon})$ can be calculated. Use of $p\left(\frac{\underline{k}}{\underline{k}}\right)$ allows a priori information to be used

The method of linear least squares produces efficient unbiased estimates if the residuals are uncorrelated and follow the same probability distribution [6,41].

(b) Weighted Least Squares [6,11,41]

The least-squares approach can be generalized by including a weighting matrix \underline{W} in the performance index:

$$S = \underline{\epsilon}^T \underline{W} \underline{\epsilon} = \sum_{i=1}^N \sum_{j=1}^N \epsilon_i w_{ij} \epsilon_j \quad (11)$$

Often the elements of the weighting matrix are selected to reflect the existing knowledge about the relative precision or importance of the residuals. This approach is particularly useful when several output variables are measured with different degrees of precision. Assume the residuals have zero means and a covariance matrix \underline{R} , i.e. $\underline{R} = E(\underline{\epsilon}\underline{\epsilon}^T)$ where E denotes the expectation operator. Then the selection of $\underline{W} = \underline{R}^{-1}$ produces a Markov or a 'minimum variance estimate' [41] which minimizes the weighted least-squares criterion S in equation (11).

(c) Maximum Likelihood [41,44,45]

This powerful approach requires that an assumption be made concerning the form of the joint probability density function of the residuals, $p(\underline{\epsilon})$. The parameters in this density function need not be specified but can be estimated along with the model parameters \underline{k} .

The likelihood function $L(\underline{k})$ is usually defined as the conditional probability, $p(\underline{y}|\underline{k})$, relating the output measurements \underline{y} to the model parameters \underline{k} :

$$L(\underline{k}) = p(\underline{y}|\underline{k}) \quad (12)$$

If the model is linear in \underline{k} and the residuals are Gaussian, it can easily be shown that [46,47]:

$$p(\underline{y}|\underline{k}) = p(\underline{\epsilon}) \quad (13)$$

and consequently $L(\underline{k})$ can be expressed as:

$$L(\underline{k}) = p(\underline{\epsilon}) \quad (14)$$

Once the form of the joint probability density function $p(\underline{\epsilon})$ has been assumed, parameter estimates are determined by maximizing $L(\underline{k})$ with respect to \underline{k} . If the values of certain distribution parameters in $p(\underline{\epsilon})$ such as means, variances, etc. are left unspecified, they also can be estimated by maximizing $L(\underline{k})$.

The maximum-likelihood analysis undergoes considerable simplification if the residuals are assumed to be uncorrelated and follow normal (Gaussian) distributions with zero means [11,14]. In this special case:

$$p(\underline{\epsilon}) = p_1(\epsilon_1)p_2(\epsilon_2) \cdots p_N(\epsilon_N) \quad (15)$$

where the density function for the i th residual is given by:

$$p_i(\epsilon_i) = (2 \pi \sigma_i^2)^{-1/2} \exp\left(-\frac{\epsilon_i^2}{2 \sigma_i^2}\right) \quad (16)$$

and σ_i^2 is the variance of ϵ_i . If the σ_i^2 are known, maximizing the likelihood function is equivalent to minimizing the weighted least-squares criterion in equation (11) with \underline{W} given by [11,14]:

$$\underline{W} = \begin{bmatrix} \sigma_1^2 & & & -1 \\ & \sigma_2^2 & & 0 \\ & & \ddots & \\ & & & 0 & \sigma_n^2 \end{bmatrix} \quad (17)$$

This selection of the matrix \underline{W} also results in a minimal variance parameter estimate [11,14].

The assumption of Gaussian uncorrelated residuals greatly simplifies the analysis but is often difficult to justify from physical considerations. It is important to note that the residual ϵ in equation (8) reflects both

modelling errors and measurement errors. While the measurement errors may follow a normal distribution to a reasonable approximation, modelling errors often are strongly correlated with the independent variables \underline{x} . For example, if a linear model is used to represent a highly non-linear system over a wide range of conditions, the residuals would be correlated with \underline{x} and consequently would not be normally distributed. Refer to [15] for an instructive example.

(d) Bayesian Estimation [6,46,47]

Bayesian estimation plays an important role in statistical decisiontheory and also provides a useful conceptual framework for parameter estimation. The Bayesian approach requires knowledge of two probability density functions: first, $p(\underline{\epsilon})$, the joint probability density function for the residuals, and second, $p(\underline{k})$, the a priori information concerning the model parameters to be used in the analysis. For example, $p(\underline{k})$ could incorporate results from previous experiments, judgemental information or constraints on the parameters arising from physical considerations [11]. If a priori information about \underline{k} is not available, it is ordinarily assumed that all values are equally likely.

A basic concern of the Bayesian approach is the calculation of the a posteriori conditional density function, $p(\underline{k}|\underline{y})$. This probability density function represents knowledge of the parameters after the measured values of \underline{y} and \underline{x} are available [46]. To evaluate $p(\underline{k}|\underline{y})$ Bayes' rule

[46,47] is used:

$$p(\underline{k}|y) = \frac{p(y|\underline{k}) p(\underline{k})}{p(y)} \quad (18)$$

Since the a priori density function $p(\underline{k})$ is assumed and $p(y|\underline{k})$ is available from equation (13), $p(y)$ can then be calculated from:

$$p(y) = \int_{-\infty}^{\infty} p(y|\underline{k}) p(\underline{k}) d\underline{k} \quad (19)$$

The evaluation of $p(y)$ may require multiple numerical integration if $p(\underline{k})$ is not available in analytical form.

After $p(\underline{k}|y)$ has been calculated, it is used to determine estimates of \underline{k} which are optimal according to some performance index. Three possible estimates are as follows [46,47]:

- (i) The most probable estimate (or unconditional) maximum-likelihood estimate, $\hat{\underline{k}}_1$, is the mode of $p(\underline{k}|y)$ since it satisfies the following relation:

$$p(\hat{\underline{k}}_1|y) = \max_{\underline{k}} p(\underline{k}|y) \quad (20)$$

- (ii) The minimal variance estimate (or conditional mean estimate), $\hat{\underline{k}}_2$, minimizes the following integral:

$$\int_{-\infty}^{\infty} \| \underline{k} - \hat{\underline{k}} \|^2 p(\underline{k}|y) d\underline{k} \quad (21)$$

This estimate is also referred to as the equal-risk estimate since it is equally probable that the true value of \underline{k} is larger or smaller than $\hat{\underline{k}}_2$. The estimate $\hat{\underline{k}}_2$ is also equal to the conditional mean, $E(\underline{k}|y)$, where E denotes the expectation operator.

- (iii) The minimax estimate (or minimum error estimates), $\hat{\underline{k}}_3$, is the median of $p(\underline{k}|y)$. It minimizes the maximum possible error, $\|\underline{k} - \hat{\underline{k}}\|$. If the range of $\|\underline{k}\|$ is $-\infty$ to $+\infty$, as in a normal distribution, the maximum possible error is also infinite and the minimax estimate has little meaning.

If $p(\underline{k}|y)$ is Gaussian, then the estimates $\hat{\underline{k}}_1$, $\hat{\underline{k}}_2$ and $\hat{\underline{k}}_3$ are identical [46,47]. Furthermore, if a uniform a priori density function $p(\underline{k})$ is assumed, the most probable estimate $\hat{\underline{k}}_1$ is identical to the maximum-likelihood estimate.

2. PARAMETERS IN ORDINARY DIFFERENTIAL EQUATIONS

Ordinary differential equations serve as a convenient mathematical model for a multitude of physical systems. Such models are mathematically tractable and are usually quite attractive from a computational viewpoint. Often the form of the differential equations is suggested from the theory, but some of the parameters must be estimated from experimental data. This parameter estimation problem is the subject of this section.

2.1 Differential Approximation

General Discussion [5,35]

Consider the mathematical model represented by equation (1). If the parameters are time invariant (i.e. $p(t) = p$) and all the state variables and their derivatives are accessible, the original estimation problem reduces to the simpler problem of determining parameters in an algebraic model. That is if the residuals are defined by:

$$\underline{\epsilon} = \dot{\underline{x}} - f[\underline{x}(t), \underline{u}(t), \underline{p}] \quad (22)$$

Then the statistical estimation methods presented in the introduction can be employed. This approach for estimating parameters in a differential equation model has been referred to as differential approximation.

Computational Techniques and Reliability Estimates [11,48]

The computational problem consists of locating the minimum or maximum of an algebraic function of the residuals (a performance index). If the model is linear with respect to the parameters, linear regression methods furnish an analytical solution [11,41,49]. Otherwise, search techniques can be used. Recent texts [36,50,51] and papers [52-58] on optimization methods should be consulted for a description of various gradient and direct-search methods. Bard [59] has made a comparison of gradient methods and reported that the Gauss-Newton approach is the most efficient. Greenstadt [60] also compares gradient methods. Marquardt's method [56]

has been popular in industrial applications. Henley and Rosen [61] present a computer programme for this method.

A thorough treatment of the estimation of the accuracy of the parameter values is presented by Booth and Peterson [57].

Experimental Techniques

In relatively few situations can the state variable derivatives be measured directly. Two examples are recycle [62] and differential reactors [63] which allow reaction rates to be obtained by direct measurement. If the derivatives are not available, they must be approximated by numerical differentiation or filtering, an unattractive prospect for noisy output data.

Applications

The excellent survey article by Bard and Lapidus [11] reviews applications to chemical reaction systems. Computational examples are presented in the text by Sage [35]. A recent application of the method to the dynamic modelling of a steam generator has been reported [64]. This technique has also been used to determine lateral stability parameters from flight data [65,66].

Kittrell et al. [67] show that a non-linear least-squares analysis is superior to the conventional linearized data analysis for a Hougen-Watson kinetic model. Non-linear least squares [67,68] is demonstrated to be useful in model discrimination.

2.2 Parameter Optimization

General Discussion [11,12,69]

A principal concern of modern control theory is the determination of optimal policies. If the parameter estimation problem is formulated as an 'optimal control problem', then a parameter estimate is desired which optimizes a selected performance index. This formulation offers the advantage that the wide variety of analytical and computational methods used in optimal control theory is also available to determine optimal parameter estimates.

Assume that the system of interest is represented by equations (1) and (2) and that the state variables (but not their time derivatives) are available. For convenience, the weighted least-squares criterion in equation (23) is selected as the performance index:

$$J = \sum_{i=1}^N \underline{\epsilon}_i^T \underline{W}_i \underline{\epsilon}_i \quad (23)$$

where the residual $\underline{\epsilon}_i$ is defined as the difference between the measured output y_i and the predicted output $h(x_i, u_i)$ at the i th sampling instant, i.e.

$$\underline{\epsilon}_i = y_i - h(x_i, u_i) \quad (24)$$

The positive semi-definite weighting matrices \underline{W}_i are often selected to reflect the relative accuracy of the output measurements [12]. The optimal parameter estimate which

minimizes J will be denoted by $p^*(t)$.

The various techniques available for solving optimal control problems have been classified by Lee [47] as either direct or indirect methods. Indirect methods derive the necessary conditions for optimality and then attempt to determine parameter estimates which satisfy these conditions. These methods will be discussed in section 2.3. Direct methods seek optimal estimates in a direct fashion through optimization of the performance index. The remainder of this section will be concerned with a particular direct method referred to as parameter optimization. Other direct methods such as dynamic programming can also be used [35,70].

Computational Techniques and Reliability Estimates

In the parameter optimization method, the optimal estimate is located by using search techniques to minimize the performance index. After an initial guess of the parameters is made, equation (1) is integrated and the performance index J evaluated. New parameter values are generated and the integration and evaluation of J is repeated. The iterative calculations continue until no further improvement in the value of J can be obtained. Unless hybrid computation [71,72] is utilized, numerical integration is usually required which can be time consuming.

Davison [73] presents a rapid algorithm for large linear dynamic systems.

For time-varying parameters, parameter optimization appears to be less promising than the estimation methods presented in sections 2.3 and 2.4.

Experimental Techniques

Either discrete or continuous measurements of the system outputs are required.

Applications

Bard and Lapidus [11], Peterson and Lapidus [74], Himmelblau et al. [75] and Mesaki and Butt [76] discuss the estimation of reaction rate constants from integral conversion data. Chen et al. [77] applied the conjugate gradient technique to the identification of aircraft parameters.

2.3 Methods Based on Optimal Control Theory

General Discussion [12,35,47,78-82]

As mentioned in section 2.2 the indirect approach for solving optimal control problems consists of deriving the necessary conditions for optimality and then attempting to determine parameter estimates which satisfy these conditions. In this section we will consider an indirect approach which has been predominant in the optimal control literature.

The derivation of the necessary conditions which $\underline{p}^*(t)$ must satisfy is easily accomplished using analytical methods such as the calculus of variations, dynamic programming or Pontryagin's maximum principle [35,70,83]. An iterative computational method is then used in which the successive estimates of $\underline{p}^*(t)$ are forced to satisfy the necessary conditions and (hopefully) will converge to $\underline{p}^*(t)$. One advantage of this indirect approach is that, in principle, the optimal estimate can be determined analytically. Unfortunately, this advantage is seldom realized since the necessary conditions inevitably require the solution of a non-linear two-point boundary value problem (TPBVP), a difficult computational problem [35].

Computational techniques for solving the TPBVP can be conveniently classified as sequential or nonsequential. In the sequential approach, parameter estimates are generated at each sampling instant t_i . Consequently, this approach is particularly well suited for on-line estimation since storage requirements are greatly reduced. In nonsequential methods the calculations are not begun until after all the data have been obtained.

Gradient methods provide a nonsequential approach which has been widely used with considerable success [35,70,84]. However, convergence of gradient techniques near the optimum estimate $\underline{p}^*(t)$ is often slow [35,70].

Second variation methods, an extension of the gradient method, converge rapidly near the optimum but required good initial estimates of $p^*(t)$. They also greatly increase the computational requirements [35,70].

Quasi-linearization is another nonsequential method that has received considerable attention [35,78,85,86,87]. Introduced into the control literature by Bellman and Kalaba [88-90], quasi-linearization is a modification of the Newton-Raphson technique for functional equations [91]. It converts the non-linear boundary value problem into a series of non-stationary linear boundary value problems. Since quasi-linearization exhibits quadratic convergence, convergence is rapid when it does occur. Unfortunately, the region of initial parameter estimates which results in convergence can be quite small. Donnelly and Quon [92,93] have proposed an algorithm to overcome the convergence problem. Gradient methods and differential approximation have been successfully used as a starter for quasi-linearization [5,35,94]. Another computational difficulty is that a set of ill-conditioned linear equations often result when the number of parameters (and unknown initial states) to be estimated is quite large [78].

In the next chapter an algorithm which combines quasi-linearization and linear programming is demonstrated to be versatile. In particular, constraints on parameters or

states are easily incorporated into the analysis and can be used to extend the region of convergence. This approach requires the selection of a linear performance index [95], rather than a non-linear index such as the least-squares criterion.

Lee [96] discusses the extension of a quasi-linearization analysis to systems with time-variable parameters.

A sequential solution to the non-linear estimation problem is also referred to as a non-linear filter since current state estimates as well as parameter estimates are generated as the output measurements become available. Most non-linear filtering techniques utilize linearization at some point in the analysis [12]. Comparisons of sub-optimal non-linear filters are available [97-99]. Invariant imbedding is a promising sequential technique that has been used in several investigations [12,35,78]. Its region of convergence is considerably larger than the region of quasi-linearization [78].

Computational Techniques and Reliability Estimates

Several recent textbooks on optimal control place considerable emphasis on computational methods [35,46,70, 100]. Review articles are available which provide an introduction to the extensive literature on optimal control theory [84,101,102] and applications to parameter

estimation [12,103-114].

Sequential estimation methods automatically generate an approximation to the covariance matrix for the parameter estimates. A thorough treatment of the reliability of parameter estimates obtained from quasi-linearization is presented by Heineken et al. [37]. Refer also to [36,115]. Reliability estimates are also easily obtained when quasi-linearization and linear programming are combined as demonstrated in Chapter 3.

Experimental Techniques

Either discrete or continuous measurements of the system output, $y(t)$, and input, $u(t)$, are required.

Applications

Sequential estimation methods have been applied to chemical reactors [2,78,116,117], paper making [118-120], navigation systems [13,104,121-123] and steel making [124]. Applications of nonsequential methods include chemical reaction systems [12,37,78,92,125,126], and biomedical systems [127,128]. It is noteworthy that several applications utilized experimental data from industrial processes [116,118,119,124]. In Chapter 3 off-line identification of a pilot plant evaporator is presented.

2.4 Model Reference

General Discussion [129-133]

In the model reference or learning model approach [134], parameters in an assumed model are adjusted until the model and plant outputs become identical. The input $u(t)$ to the plant is measured and fed to the model; the difference between the measured plant output and the model output is used in an adaptive loop to adjust the model parameters (see Figure 1). The parameter adjustment is usually done on a sequential basis but could be done non-sequentially [135]. Model reference methods have received considerable attention as indicated by the large number of papers in recent I.F.A.C. symposia.

The model reference approach has also been widely used to design adaptive control systems [133]. Since the adaptive control and identification problems are 'dual problems', the parameter-adjustment algorithms developed for adaptive control can also be used for identification [133,136,137]. The simplicity and sequential nature of the model reference approach make it attractive for on-line applications such as tracking time-varying parameters. However, convergence to the actual parameter values and an acceptable rate of convergence may be difficult to guarantee [136,138].

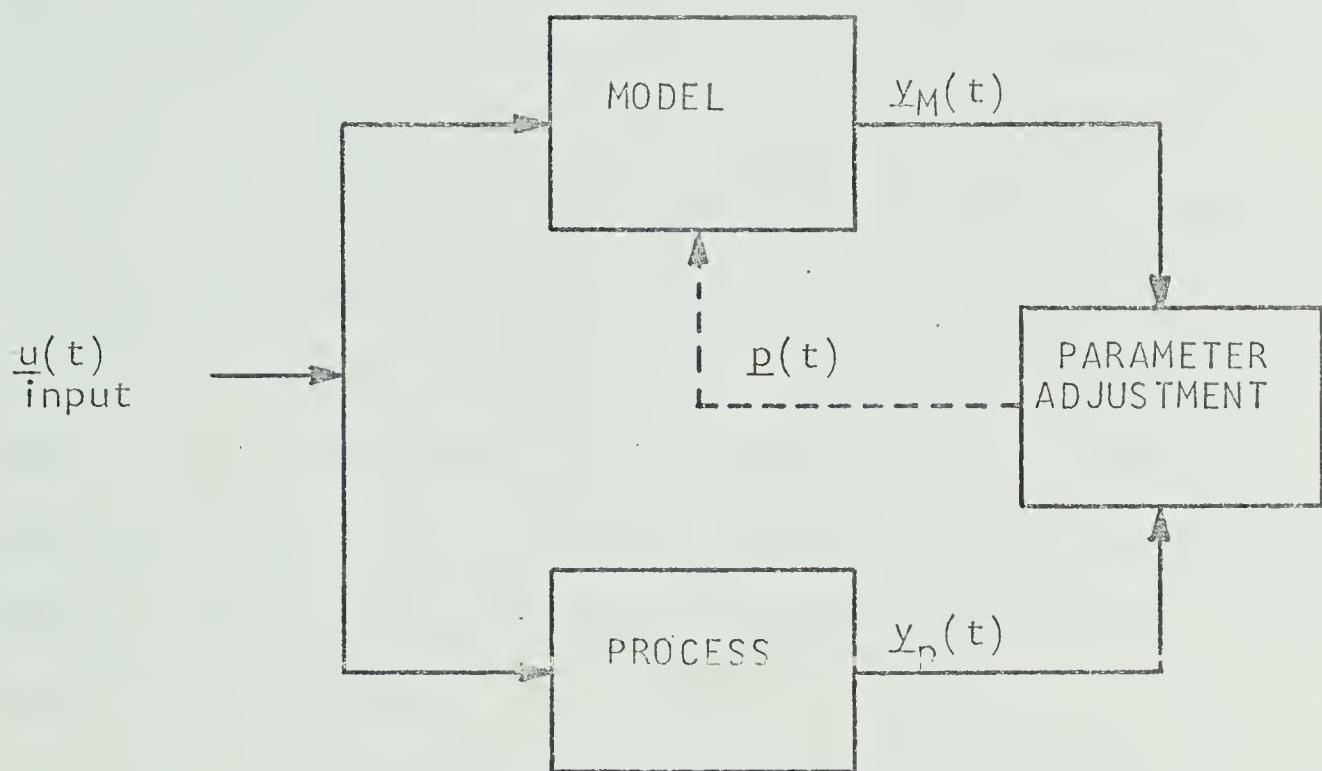


FIGURE 1: Model Reference Approach to Parameter Estimation

Computational Techniques and Reliability Estimates [139-142]

Two design strategies have received the most attention. In the first approach, the parameter-adjustment scheme is designed to minimize a performance index based on the process and model outputs. Popular performance indices have included the integral squared-error criterion and algebraic functions of the instantaneous outputs and their time derivatives [130, 143-147]. Certain difficulties associated with algebraic performance indices have been noted by several authors [130, 143, 147]. The required minimization is typically achieved by using gradient techniques [130, 147-149] or the related method of stochastic approximation [150-157] to develop a parameter adjustment law of the following form:

$$\frac{dp}{dt} = -K \nabla_{\hat{p}} [J(\underline{e})] \quad (25)$$

$J(\underline{e})$ = scalar performance index,

\underline{e} = output error = (model output) - (plant output),

$\nabla_{\hat{p}}$ = gradient with respect to the adjustable model parameters, \underline{p} ,

K = constant matrix.

The gradient has often been evaluated from sensitivity equations [7, 130, 132, 143, 158-161]. The use of 'state-variable filters' [147, 162] can improve stability and convergence properties.

A second popular approach is to use Liapunov's second method to ensure the stability of the resulting model reference system. This approach has enjoyed considerable success for multivariable linear systems [163-166]. However, at present the resulting parameter-adjustment algorithms require all state variables to be accessible. Landau [167] has demonstrated that Popov's method also provides a systematic approach for designing globally stable adaptive systems.

A less attractive approach is to competitively rate a collection of models. However, large computer times are necessary [5,168].

Experimental Techniques

Some model reference algorithms require all state variables to be measured; other algorithms require only output measurements.

Applications

The problem of auto-pilot design motivated much of the early work in this field [133]. The survey article of Maslov and Osovskii [169] lists applications of the model reference approach in chemical and metallurgical processes, aeronautics and electrical engineering. Refer also to the text by Eveleigh [133] and additional survey articles [129, 132]. A model reference control system has also been reported for nuclear rocket engines [170]. Bell [171] pre-

sents a hybrid computer study of a model reference parameter-tracking system. Porter and Tatnall [172] report the performance of an adaptive hydraulic servomechanism.

2.5 Step Response

General Discussion [173,174]

Low-order, single-input, single-output systems are often characterized by 'time constants' which indicate the speed of response of the system. The transient response to a step change in an input variable can be used to determine these time constants and time delay, if any, which characterize the system. This method has been widely used since it is simple to apply and easy to interpret. However, the test is very sensitive to other disturbances [7,175]. This method is often used when approximating a higher-order system by a second-order model with a time delay [176].

Computational Techniques and Reliability Estimates

The Oldenbourg-Sartorius method and the slope intercept (or percentage incomplete) method can be used to estimate time constants [173,174]. These simple, graphical methods eliminate the need for machine computation. The parameters can also be determined by curve fitting the response data [177-179]. If the system is approximated by a first-order lag plus dead time, the parameters can be obtained directly from a plot of the step response [175].

Experimental Techniques [173,180]

A step change in an input variable is introduced and the transient response is recorded. Attempts have been made to reduce experimental time by trajectory extrapolation [181].

Applications

Cheruy and Menendez [175] made an experimental comparison of step, pulse and random signal testing using an electric furnace. Bakke [182] used a "modified step response method" to determine the parameters in a first-order plus delay model of a pilot plant distillation unit. Laspe [178] investigated the dynamic behaviour of an oil-cracking furnace.

2.6 Repeated Integration

General Discussion [183,184]

In this approach, repeated integration of input and output data is used to estimate parameters in time-invariant linear systems. For purposes of illustration, consider the following nth-order single-input, single-output system where the a's and b's are unknown parameters ($n > m$):

$$\begin{aligned} b_n \frac{d^{(n)}y}{dt^n} + \dots + b_1 \frac{dy}{dt} + y(t) \\ = a_m \frac{d^{(m)}u}{dt^m} + \dots + a_1 \frac{du}{dt} + a_0 \end{aligned} \quad (26)$$

If equation (26) is integrated numerically n times from 0 to T , an algebraic equation which is linear in the a 's and b 's results [183]. Since there are $n + m + 1$ parameters to be identified, either $n + m + 1$ experimental output responses are required or a single output response can be used if the repeated integrations are performed for $n + m + 1$ different time intervals. In either case, if the resulting set of $n + m + 1$ algebraic equations is linearly independent, the a 's and b 's can easily be determined.

This approach to parameter estimation has mainly been used for linear systems. However, Diamesis [185], Wang [186] and Radtke [187] have extended this method to systems with polynomial non-linearities.

Computational Techniques and Reliability Estimates [188,189]

A major source of difficulty is encountered in obtaining a set of independent linear algebraic equations. If response data from a single experimental test are to be used, Murrill et al. [183] recommend taking at least $5n$ data points. If results from several experimental tests are to be used, the forcing function (inputs) must be linearly independent.

Experimental Techniques

An arbitrary disturbance is introduced into the system via the input $u(t)$. The input and output $y(t)$ are recorded at every sampling instant.

Applications

Heimlich and Gruet [190] applied this method to a fluidized bed system. Schneider [191] used this technique for process identification in an adaptive feed-forward control scheme.

3. PARAMETERS IN AN ANALYTICAL SOLUTION

The most time-consuming computational step in most of the methods for estimating parameters in differential equations (cf. section 2) is the integration of the model equations which must be done for each iteration of the parameter estimation procedure. This integration step can be avoided if an analytical solution exists for the system equations. For example, the time-varying, multi-variable, linear system described by equation (3) has the solution [192]:

$$\underline{x}(t) = \underline{\phi}(t, t_0) \underline{x}(t_0) + \int_{t_0}^t \underline{\phi}(t, \xi) \underline{B}(\xi) \underline{u}(\xi) d\xi \quad (27)$$

where the fundamental or transition matrix is defined by:

$$\frac{d}{dt} \underline{\phi}(t, t_0) = \underline{A}(t) \underline{\phi}(t, t_0) \quad (28)$$

with

$$\underline{\phi}(t_0, t_0) = I \quad (29)$$

For time-invariant systems the solution is considerably simpler and is given by equation (7).

The estimation problem is now to determine the unknown parameters in the transition matrix given measured values of the system input, $u(t)$, and output $y(t)$. No integration is required but the estimation problem is non-linear and the solution may be difficult since some of the parameters will occur in the arguments of exponential or transcendental functions as discussed in section 1.1 (b).

This approach is frequently used in low-order, or single-input, single-output systems and usually requires simplifying assumptions which permit an analytical solution to be obtained or which reduce it to a set of estimation problems which can be solved independently or sequentially. Many reaction kinetics and catalysis mechanism problems fall into this category.

Heymann et al. [193] present a time-domain technique for the identification of linear, time-invariant, single-output, single-input systems. The model is identified using a pseudo-state-space formulation and a two-stage solution procedure which identifies the system poles (i.e. weighting function or fundamental matrix) and then the 'complete model' (i.e. poles, zeros and lags). The second

step involves analytic differentiation of the weighting function and solution of a set of linear algebraic equations. The principal advantages are that the solution is all in the time domain, repeated integrations rather than differentiation of the response data are used, and the method evaluates confidence limits simultaneously with the parameter estimates. For an nth-order system, n linearly independent response functions are required and in practice this limits the model to relatively low orders. The authors report applications to second and third-order systems simulated on an analogue computer, an operating chemical plant and a stirred tank heat exchanger. They conclude that this is a useful technique for linear systems and has 'modest' computational requirements.

3.1 Search Techniques

General Discussion

The parameter estimation problem is analogous to that of section 2.1 where the object is to minimize a function of the residuals with respect to the parameters, p .

Computational Techniques [194] and Reliability Estimates [11,57]

In the general case, non-linear estimation techniques are required and the search techniques discussed in section 2.1 are applicable. However, numerical or analogue inte-

gration techniques need not be incorporated since the analytical solution is available in closed form.

Experimental Technique

Transient data are recorded for known or measured disturbances and the trajectories are fitted, usually by least squares. State derivatives are not required.

Applications

Ball et al. [195] apply this method to reaction kinetic systems. Berry [196] uses Rosenbrock's method of rotating coordinates [36] to identify parameters in the solution to low-order models of a pilot-plant binary distillation column. Latour et al. [177] employ Marquardt's method to determine the parameters in a second-order model used for control purposes. Moore et al. [197] use a pattern-search technique.

3.2 Prony's Method of Exponential Approximation

General Discussion

The homogeneous solution for a nth order, linear, time-invariant, single-output system, can be written in the following form:

$$y(t) = \sum_{i=1}^n K_i t^j \exp(\lambda_i t) \quad (30)$$

where eigenvalues, λ_i , may be repeated r times ($0 \leq j \leq (r-1)$)

The calculation procedure to identify the parameters K_i and λ_i involves two linear regressions and the determination of the roots of an nth-order polynomial. However, non-linear regression and integration of the system differential equations is avoided.

Computational Techniques [198] and Reliability Estimates

Denoting the sampling time as T , $y(kT)$ as y_k and $\exp(\lambda_i T)$ as α_i it can be shown [199] that

$$y_{m+n+1} = \sum_{i=1}^n w_i y_{m+i}, \quad m = 0, 1, 2, 3, \dots, M \quad (31)$$

where w_i is dependent only upon λ_i and T and can be identified by using least-squares techniques to fit equation (31) to experimental data where $M \geq n$, and the number of data points is greater than $M + n$.

Once the w_i values have been determined the values of α_i can be found by finding the roots of the following polynomial [199]:

$$\alpha^n = \sum_{i=1}^n w_i \alpha^{i-1} \quad (32)$$

and λ_i follows from

$$\alpha_i = \exp(\lambda_i t) \quad (33)$$

Since the modes, α_i , are now known the values of K_i can be determined by fitting equation (30) to the data using techniques such as linear least squares.

Experimental Technique

Transient responses of the system output, $y(kT)$, are recorded for sets of initial conditions which must be chosen to excite all desired modes of the system.

Applications

Chidambara [200] uses this technique for the reduction of an eighth-order model by assuming a model of order four and determining the parameters which give the best 'fit' to data generated by the eighth-order model. It should be noted that this method of model reduction does not necessarily preserve the dominant eigenvalues of the original system. Meier and Luenberger [201] use Prony's method as a starter for the Wiener filter.

4. PARAMETERS IN A DISCRETE MODEL

Discrete models have received a great deal of attention recently because of the rapidly increasing use of digital computers for on-line data acquisition and/or data processing. All of the models represented by equations (1) to (6) can be put into discrete form by replacing the continuous variable, t , by kT where T is the sampling interval and k assumes integer values. (In this work it is assumed that T is constant and is normally omitted, so that $x(t) = x(k) = x_k$ implies that $t = kT$).

Estimation of the parameters in the discrete form of equations (1) and (2) usually requires linearization at some stage of the analysis [12,35].

Treatment of the discrete linear system derived from equations (3) and (4) involves manipulation of the equations so as to obtain a difference equation which relates the output to the input [22,35,77].

The linear, time-invariant case can be easily treated analytically. Under the assumption that $\underline{u}(t)$ is constant over the sampling interval, it can be shown [192] that the analytical solution to the discrete form of equations (5) and (6) is:

$$\underline{x}(k+1) = \underline{\phi}\underline{x}(k) + \underline{\Delta}u(k) \quad (34)$$

$$\underline{y}(k+1) = \underline{G}\underline{x}(k) + \underline{v}(k) \quad (35)$$

It must be emphasized that this is not a numerical approximation and agrees exactly, at the sampling instants, with the solution of the equivalent continuous model.

The parameter estimation problem associated with equations (34) and (35) is to find numerical values for the elements of the $\underline{\phi}$ and $\underline{\Delta}$ matrices [202,203]. Thus, in this sense the problem is analogous to section 3 which dealt with estimating parameters in the solution to a differential equation. However, since $\underline{\phi}$ and $\underline{\Delta}$ are analytical functions of \underline{A} and \underline{B} it is also possible to work back and find

the parameters in the original differential equations as discussed in section 1.1. An alternative discrete representation for a multivariable dynamic system is:

$$\underline{A}z(z^{-1}) \underline{y}(t) = \underline{B}z(z^{-1}) \underline{u}(t) \quad (36)$$

where

- n = order of the state vector
- m = dimension of the input vector ($m < n$)
- z = z transform variable
- $\underline{A}z$ = matrix of polynomials of order n
- $\underline{B}z$ = matrix of polynomials of order m

The single variable form of equation (36) is widely used and can be written in terms of the pulse transfer function, $G(z)$:

$$G(z) = \frac{y(z)}{u(z)} = \frac{z^{-q} \sum_{i=0}^m b_i z^{-i}}{\sum_{i=0}^n a_i z^{-i}} \quad (37)$$

where q is a time delay parameter and z is the transform variable such that z^{-i} indicates a pure time delay of i sample periods. Thus, in the time domain equation (37) becomes:

$$\sum_{i=0}^n a_i y(k-i) = \sum_{i=0}^m b_i u(k-i-q) \quad (38)$$

where k is the time interval of interest.

The estimation problem is then to estimate the parameters a_i and b_i given a time series of data for y and u . It should be noted that one coefficient can be eliminated by dividing both sides of the equation by, say b_0 .

The above equations were derived from the state space or matrix models of the system. An alternative approach which is widely used, and particularly suitable for linear control systems, is based on 'block diagram' and 'transfer function' written in terms of the Laplace variable, s , or the z-transform variable, z . Digital simulation programmes are available which also convert from the Laplace transform to an equivalent state-space formulation [204] or to handle mixtures of Laplace and z-transforms [205]. These methods can be used [206] for determining discrete approximations (in the form of equation (36) or (38)) for continuous systems. The advantage lies in faster evaluation of the transients from the system model and is particularly important for real-time digital simulation studies. The ratio of computation speeds achieved by discrete approximation vs. numerical integration methods - for the same accuracy - has been more than a hundred to one in some cases [206].

Some of the methods based on optimal control theory (section 2.3), such as quasi-linearization [207,208], can be formulated to apply to discrete systems.

4.1 Statistical Estimation

General Discussion [14]

In discrete model formulations such as those represented by equations (34) to (38) the problem is reduced to the estimation of parameters in an algebraic equation and a wide variety of methods is available.

Computational Techniques and Reliability Estimates [38,209-211]

The method of linear least squares which provides a convenient method of analysis if the model is a true regression model leads to estimates which are biased and non-minimum variance when both $y(t)$ and $u(t)$ are corrupted by noise [14,212]. The bias caused by the noise can be easily compensated for if the noise properties are known. However, this is not the situation in most practical problems and other approaches [213-215] must be employed at the expense of increasing the complexity of the analysis. Other pitfalls of linear regression were related by Young [213] and Box [212].

Least squares [214,216-220] and maximum likelihood [221-227] have been applied extensively to single-input, single-output models. Other techniques [228-233] convert discrete problems to the s domain by matching root loci of the discrete and continuous system.

Similarly for multi-input, multi-output systems least squares [13,118-120,124], maximum likelihood [234-235] and the instrumental variable method [13,162,236] are

employed.

So as to facilitate on-line identification of the discrete model, recursive schemes have been presented for both single-output [237-240] and multi-input, multi-output [241-245] process identification.

Use of the Cramer-Rao inequality has been made by Astrom [38] to provide an estimate of the reliability of the parameter estimates.

Experimental Technique [246]

Discrete time series data are needed for the inputs and outputs. A pseudo-random binary test signal is a very popular forcing function [214]. Williams and Clarke [247] present a state-of-the-art paper on the use of pseudo-random binary sequences. Menahem [248] employs a multi-step test signal.

Applications [246]

Astrom [215] presents an application of computer control of a paper-making process which involves identification by this scheme. Other applications to the paper industry include [118-120,226,249,250]. Wilkie [251] applies generalized least-squares and maximum-likelihood estimation to a small nuclear reactor. Computation times are reported. Other applications are to a distillation column [252], a steel-making process [124], determination of aerospace vehicle parameters [253,254], oil refinery unit

[255], a paper machine [256], aeronautics [251] and a thermal process [258].

4.2 Kalman Filtering

General Discussion [259-261]

In general, the term 'filtering' can be applied to any procedure which produces an updated estimate of the desired quantity at each sampling instant. The classical approach to state estimation derived by Kalman [261] provides minimum-variance, unbiased estimates of the state, $\underline{x}(t)$ (for systems described by equations (3) and (4)), based on measurements of the output vector, $y(t)$. The linear filter is stable for systems that are observable and controllable.

Estimates of unknown parameters can be obtained by augmenting the state matrix so that it contains the described parameters as follows:

$$\underline{z}(t) = \begin{bmatrix} \underline{x}(t) \\ p(t) \end{bmatrix} \quad (39)$$

and then applying state estimation techniques [260]. The 'augmented models' follow directly from equation (1) to (6) by replacing $\underline{x}(t)$ by $\underline{z}(t)$.

There is no general solution for the non-linear filtering problem. Therefore, most techniques rely on local linearization to yield a sub-optimal filter such as the

'extended Kalman filter'. However, in this instance there is no guarantee of stability of the filter.

For systems which can be adequately represented by the following equations:

$$\underline{z}(k+1) = \underline{f}_1(\underline{z}(k), k) + \underline{B}(k) \underline{u}(k) \quad (40)$$

$$\underline{y}(k+1) = \underline{C}(k) \underline{z}(k) + \underline{v}(k) \quad (41)$$

the extended Kalman filter has the following form [46]:

$$\underline{P}(k+1) = \underline{E}_{\underline{z}}[\hat{\underline{z}}(k)] \underline{H}(k) \underline{E}_{\underline{z}}^T[\hat{\underline{z}}(k)] + \underline{B}(k) \underline{Q} \underline{B}^T(k) \quad (42)$$

$$\underline{H}(k) = \underline{P}(k) - \underline{P}(k) \underline{C}^T(k) (\underline{R} + \underline{C}(k) \underline{P}(k) \underline{C}^T(k))^{-1} \underline{C}(k) \underline{P}(k) \quad (43)$$

$$\hat{\underline{z}}(k+1) = \underline{f}_1[\hat{\underline{z}}(k), k] + \underline{H}(k) \underline{C}^T(k) \underline{R}^{-1} (\underline{y}(k+1) - \underline{C}(k+1) \underline{f}_1[\hat{\underline{z}}(k), k]) \quad (44)$$

where $E[\underline{u}(k)] = E[\underline{v}(k)] = 0$ and

$$\underline{E}_{\underline{z}}[\hat{\underline{z}}(k)] = \frac{\partial \underline{f}_1}{\partial \hat{\underline{z}}(k)}$$

which is simply equal to $\underline{\phi}(k)$ for the linear system. The matrices \underline{Q} and \underline{R} are defined as covariance matrices of the uncorrelated random inputs $\underline{u}(k)$ and $\underline{v}(k)$ respectively.

$\underline{H}(k)$ is an a posteriori covariance matrix in the algorithm.

Suboptimal filter equations can also be derived using invariant imbedding [12,263-265]. For time-invariant linear systems the Wiener filter is applicable and requires significantly less computational effort [266].

It should be noted that this formulation of the parameter-estimation problem results in a non-linear set of difference equations (which must be solved at each time interval) even for models that are linear in the augmented state vector.

Computational Techniques [117,260,267-272] and Reliability Estimates

An estimate of the initial value of the augmented state vector, $\underline{z}(0)$, an estimate of the covariance matrix, $\underline{P}(0)$, and an estimate of the covariance matrices \underline{Q} and \underline{R} are required to initiate the filter. The algorithm is summarized in equations (42) and (44). Decomposition of the state vector has been studied to reduce the computational load [273].

Calculation of the covariance matrix of the augmented state vector is inherent in the algorithm. However, for the extended Kalman filter the estimates of the parameters are biased and there is no guarantee that $\underline{P}(k)$ will converge [117,260,274]. The performance of the Kalman filter when the model is imperfect and the noise statistics poorly defined has been studied [275,276].

Experimental Techniques

The method is sequential and requires the solution of equations (42) to (44) at each sample time. Therefore, an on-line process computer is required to implement this scheme.

Applications [269]

Application of the technique to a six-dimensional non-linear stirred tank reactor is related by Wells [117] in an excellent presentation. Other applications include a paper machine [118,119], a reactor system [116,277,278], orbit parameter estimation [279] and guidance [269].

5. COEFFICIENTS IN A FUNCTIONAL SERIES EXPANSION

Expansion of the system output as a functional power series of the input is a time-domain technique which can be applied to non-linear systems and does not require any a priori knowledge of the structure of the system. Aleksandrovskii and Deich [10], in a comprehensive review of the literature on methods for determining the dynamic characteristics of non-linear systems, conclude that the functional power series representation is the most promising approach. However, as normally formulated for non-linear systems this approach is generally poor for linear systems due to the non-linear nature of the component functionals. To date this technique has been mostly of academic interest due to the large computational times required.

It should be emphasized that this approach simply produces an input-output relationship in the form of a series. Transformation of the results into an alternative mathematical representation such as a set of differential equations or multi-dimensional frequency response or transfer functions is difficult and sometimes impossible. The synthesis of the system model is, in practice, not unique since many systems with different physical configuration can exhibit the same transmission (input-output) characteristics. Nevertheless, the resulting explicit relationship allows the system output, $y(t)$, to be calculated for any specified input, $u(t)$, and is useful in simulation studies and some design techniques.

5.1 Volterra Expansion

General Discussion [280-283]

A large class of continuous, non-linear, time-variant systems can be represented by a Volterra series expansion of the form:

$$y(t) = \sum_{n=1}^{\infty} \int_0^{\infty} \dots \int_0^{\infty} g_n(t, \tau_1, \tau_2, \dots, \tau_n) \prod_{i=1}^n u(t - \tau_i) d\tau_i \quad (45)$$

Equation (45) is an extension to non-linear systems of the classical convolution integral representation of linear systems discussed in section 6. In the general case the multi-variate kernel in equation (45) reflects the dependence

of the transient process on the input signal amplitude and the past state of the system. If the process response, $y(t)$ is not significantly affected by the inputs which occurred prior to some time, $t - mT$, the process is said to have a 'finite memory' and the series in equation (45) can be truncated to a finite number of terms, N . Under certain conditions, convergence of the series is assured by the Freche theorem and estimates for the convergence of the series can be obtained [10,284].

Solution of the identification problem requires determination of the kernels $g_1(t, \tau_1) \dots g_n(t, \tau_1 \dots \tau_n)$ in equation (45). Methods for direct calculation of the kernels have been proposed but the more common approach is to approximate the kernels by an expansion in terms of orthogonal functions, such as the following:

$$g_n(t, \tau_1 \dots \tau_n) = \sum_{n=0}^N \sum_{m=0}^N \dots \sum_{k=0}^N a_{nm\dots k} \phi_n(\tau_1) \phi_m(\tau_2) \dots \phi_k(\tau_n) \quad (46)$$

After selection of a suitable set of orthogonal functions the identification problem is reduced to the determination of the parameters $a_{nm\dots k}$ which in general cases may be functions of time. Alexandrovskaia and Deich [10] have reported on algorithms for the statistical determination of these coefficients based on the criterion of root-mean-square error.

The integrations in equation (45) can be approximated by an equivalent series of summations to produce a discrete or sampled data formulation of the same technique.

Computational Techniques [10] and Reliability Estimates

Unfortunately, the technique, inspite of the simplicity of the concept, results in a large number of coefficients which must be estimated. Proper choice of the orthogonal functions and the input signal can reduce the dimensionality of the estimation. Current methods of solution include the gradient-type methods [285-288], pattern-recognition techniques [289,290] and others [291-294]. In theory this concept can be implemented on-line and can be extended to multi-variable systems.

Experimental Techniques [295]

The input to the system is arbitrary and the form of $u(t)$ may be chosen by the user. However, Wiener [296] has shown that the optimum test signal for non-linear system analysis is Gaussian white noise. Many of the binary sequences [246,297] provide a satisfactory model of white noise and are easier and more convenient to implement.

Applications

Kwatny and Shen [298] solve two numerical examples. Lubbock and Barker [288] use analogue techniques to identify a heat exchanger. Katzenelson and Gould [291] are partially successful in applying this technique to char-

acterize the servo-mechanism associated with the pupil of the human eye.

5.2 Wiener Theory

General Discussion [9,281,299-303]

Wiener's method consists, essentially, of subjecting an unknown non-linear system to a Gaussian white-noise input and calculating the cross-correlation of its output with non-linear functions of its input. The technique follows directly from orthogonalization of the Volterra expansion (cf. section 5.1) [10] and is covered thoroughly by Harris and Lapidus [9].

The method is limited to stable systems with finite memory and the physical characteristics of the process are not considered. The result is simply a functional relationship between the system output and its input.

If the past of the input time function can be characterized by expansion in a complete set of orthonormal functions, $\phi_i(t)$, such that

$$u(t) = \sum_{i=0}^{\infty} c_i \phi_i(t) \quad (47)$$

then the coefficients of the functional expansion, c_i , determine $u(t)$ and form a spectrum by which the analyzed function can be identified. Wiener selected a Laguerre

function expansion because of its mathematical properties and the fact that the characterizing coefficients can be generated by analogue means.

The value of the system output, $y(t)$, can then be represented by an arbitrary, orthogonal expansion in terms of the input $u(t)$. However, since $u(t)$ can be characterized by the coefficients, c_i , of equation (47), it is possible to express the output series expansion as a function of c_i . Selecting Hermite polynomials, ψ_i , for the expansion because they are orthogonal with respect to a white Gaussian process permits simplification of the expression for the system output to the following form

[9]:

$$y(t) = \lim_{n \rightarrow \infty} \sum_{i_0=0}^{\infty} \dots \sum_{i_n=0}^{\infty} a_{i_0 \dots i_n} \psi_{i_0}(c_0) \dots \psi_{i_n}(c_n) \quad (48)$$

The coefficients, $a_{i_0 \dots i_n}$ of the series (48) appear linearly and because of the orthogonal nature of the model can be evaluated independently and have the important property of 'finality', i.e. $y(t)$ from equation (48) can be made to approximate the experimental response to any degree of accuracy by increasing the number of Laguerre coefficients and addition of the $(n+1)^{st}$ Hermite coefficient does not necessitate re-evaluating the previously

determined n coefficients. Practical application of Wiener's method is limited by the large number of coefficients to be evaluated and the sophisticated (preferably hybrid) computing facilities required to analyse the results.

Computational Techniques [9,10,304] and Reliability Estimates

In practice only a finite number of coefficients in the functional expansions can be evaluated and error analysis is difficult. The extension to Wiener's method by Bose [305-306] leads to more practical implementation. Harris and Lapidus [9,307] and Roy et al. [308] apply this method to models of non-linear, time-invariant processes with switched two-level inputs and finite memories.

Experimental Technique

A Guassian white-noise test signal, or one of its approximations, is applied over a relatively large period of time. The technique is off-line in practice because it is convenient to use the recorded data of $u(t)$ and $y(t)$ repeatedly in the serial evaluation of the coefficients.

Applications

No 'physical' applications are reported. Harris and Lapidus [9,307,309] use digital computer simulation to apply the method to a stirred tank reactor. Wilkie [251] compares this method with several other techniques for application to the identification of a small nuclear reactor.

6. IMPULSE RESPONSE

The impulse response can be defined as the response of the system output variable to a Dirac delta function input, i.e. an input pulse of height, h , and duration, $1/h$, in the limit as h tends to infinity. However, the impulse response is seldom found by such direct testing and its importance lies with its association with classical Laplace transform analysis and because the response of a linear system to any arbitrary forcing function can be calculated if the impulse response is known (equations (50) and (51)).

For time-invariant, linear single variable systems the input-output relation in the Laplace domain, assuming zero initial conditions, is:

$$y(s) = G(s) u(s) \quad (49)$$

Formal application of the convolution theorem yields:

$$y(t) = \int_0^t g(t - \tau) u(\tau) d\tau \quad (50)$$

Since the Laplace transform of the impulse function is unity, it follows directly that the impulse response, $g(t)$, can be interpreted as either the inverse Laplace transform of the system transfer function, $G(s)$, or as the system time domain response to an impulse function.

For linear multi-variable systems with zero initial conditions it follows from equation (3) that

$$\underline{y}(t) = \underline{C} \int_0^t \underline{\phi}(t, \tau) \underline{B}(\tau) \underline{u}(\tau) d\tau \quad (51)$$

Therefore, the 'impulse response' is related to the system transition matrix, $\underline{\phi}(t, \tau)$, by:

$$\underline{q}(t - \tau) = \underline{\phi}(t, \tau) \underline{B}(\tau) \quad (52)$$

For non-linear systems equation (45) can be considered as a generalization of equation (50).

Since it is impractical, in some instances, to obtain the impulse response of a system directly, several methods have been developed to calculate it, given known values of the input and output variables [310-311].

6.1 Direct Impulse Testing

General Discussion [183,312,313]

The Dirac delta function is an ideal interrogation function for system testing because it has a uniform frequency content and hence will excite all the system modes.

Computation Technique and Reliability Estimates

The impulse response is obtained directly by curve fitting an assumed process model to the observed system response [314]. The accuracy of the method is directly

dependent on how closely the system input approximates an ideal impulse. The method is generally more accurate at higher frequencies than a step test (cf. section 2.5), but is sensitive to other process disturbances and noise.

Experimental Technique [183,315]

An impulse is applied to the system input and the output response is recorded. However, in many physical systems it is impossible to generate a suitable impulse in the input variable and one of the indirect methods of obtaining the impulse response must be used.

Applications

Application to a stirred tank reactor is reported [183,315]. Tracer studies to determine the degree of mixing in a system are analogous to this technique (see section 6.4).

6.2 Deconvolution

General Discussion [5,312]

For many systems, given records of the system inputs and outputs, it is possible to calculate the impulse response from equation (50) or (51) by 'numerical deconvolution'. The data must be relatively noise-free and the process model simple if the computations are to be stable [316,317].

Computational Techniques and Reliability Estimates

Techniques for the determination of the kernel in an integral equation such as (50) or (51) by numerical deconvolution have been reported by several authors [312,318-322].

Alternatively, in a manner analogous to that of section 5.1, it can be assumed that the impulse response can be satisfactorily approximated by an infinite series of orthonormal functions and the coefficients calculated from the experimental data [323-326]. However, a large number of terms is often required for sufficient accuracy and the success of the method may depend on proper choice of the orthonormal functions.

Equation (50) can also be converted to a set of linear algebraic equations in g by the following discrete approximation:

$$y_k = \sum_{j=0}^K g_j u_{k-j} \quad (53)$$

where the subscripts define the time interval [220,327-330]. Solution of equation (53) produces the impulse response as a discrete time series which can be used directly or fitted with a suitable model.

Experimental Technique

The method does not require any particular form for the test signal but is very sensitive to noise and unmeasured disturbances.

Applications

This technique has been applied to the identification of a boiler [331].

6.3 Correlation Techniques

General Discussion [332-335]

This approach is attractive because arbitrary or random test signals can be used. It is based on the well-known Wiener-Hopf equation which relates the cross-correlation function, $\phi_{uy}(t)$, the input autocorrelation function, $\phi_{uu}(t)$, and the impulse response function, $g(t)$:

$$\phi_{uy}(t) = \int_{-\infty}^{+\infty} g(\tau) \phi_{uu}(t - \tau) d\tau \quad (54)$$

where

$$\phi_{uu}(t) = \lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^{+T} u(t)u(t+\tau) d\tau \quad (55)$$

$$\phi_{uy}(t) = \lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^{+T} u(t)y(t+\tau) d\tau \quad (56)$$

The convolution integrals in equations (54) to (56) are time consuming to evaluate for the general case but can be simplified considerably by proper choice of the input function, $u(t)$. For example, the autocorrelation function of Gaussian signals approaches a delta function so that equation (54) can be reduced to:

$$\phi_{uy}(t) = Ag(t) \quad (57)$$

where A is the root-mean-square value of $u(t)$.

The approach has been extended to multi-variable systems [336-339] and Briggs et al. [340] discuss the extension to non-linear systems.

Computational Techniques [327,341-345] and Reliability Estimates [346-353]

The deconvolution techniques of section 6.2 can be applied directly to equation (54). However, if a suitable random signal is used, then equations (56) and (57) can be applied and the calculation is simple, direct and less sensitive to noise.

Davies [354] describes a method of estimating output drift which improves the accuracy of the impulse response.

Experimental Technique

A broad-band, random test signal is preferred [355]. The pseudo-random binary sequence is simpler to generate than white noise (particularly with on-line digital computers) and allows shorter experimental times as well as

greater accuracy [348,356,357].

The set-up of the experimental test is illustrated in Figure 2. Commercial, special-purpose instruments are available [358] to perform the analysis.

Cummins [359-360] discusses the sources of errors in determining the impulse response of a process.

Matched filters have also been used in this context [361,362].

Applications

Godfrey [363] and Briggs et al. [340] list several applications. Applications include an evaporator [364], a pilot scale distillation column [365], a diesel engine [366], a heat exchanger [360,367], a gas chromatograph [368], a nuclear power plant [369], a paper machine [370], a thermal process [371], a blast furnace [372], a cardiovascular system [373] and a control system with time delays [374].

Hill and McMurry [375] present a method for on-line impulse response identification applied to several numerical examples.

6.4 Method of Moments

General Discussion [376]

"The transfer function for any stable, linear, one-dimensional system can be evaluated from experimental residence time distribution data obtained by the use of the

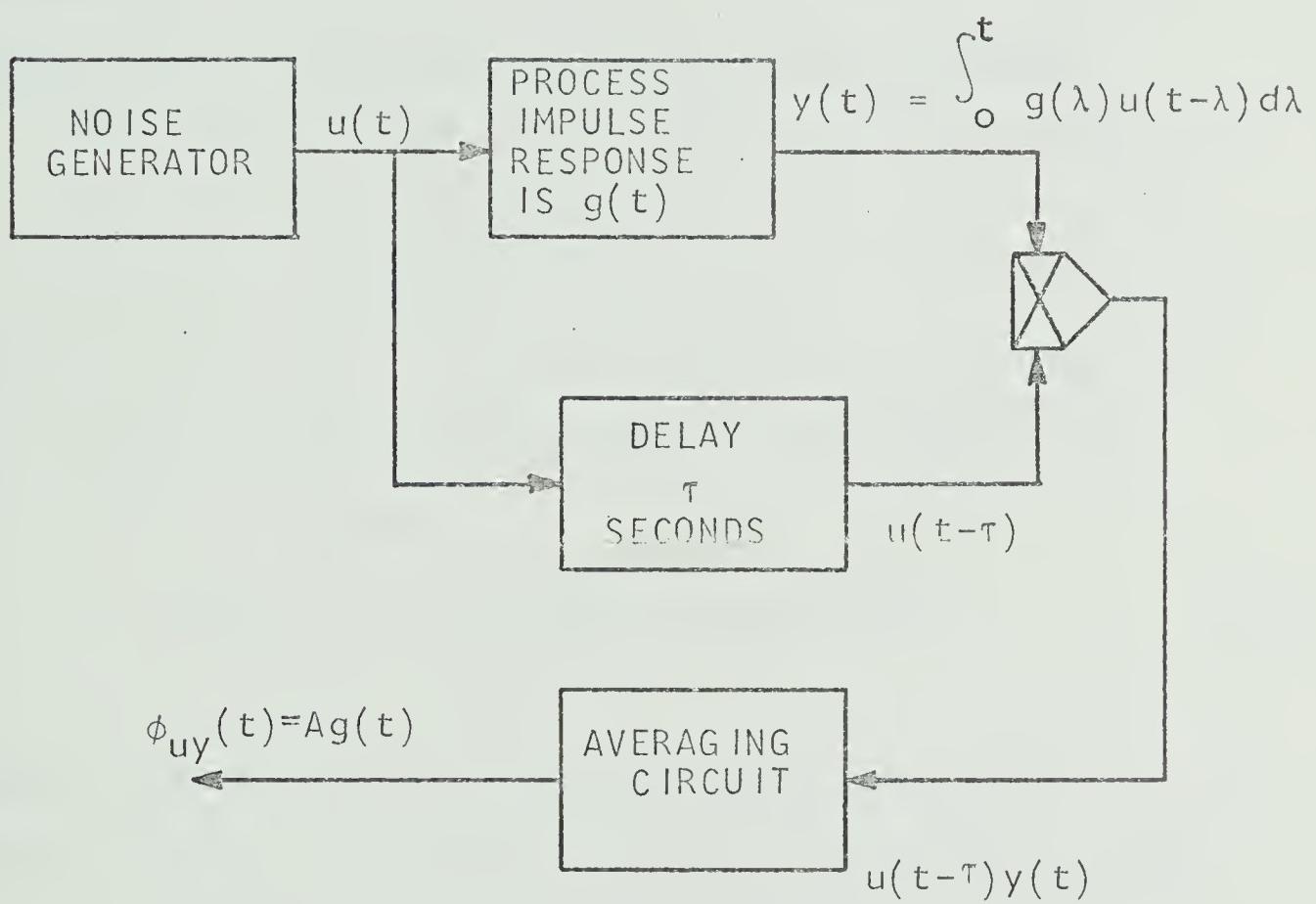


FIGURE 2: Identification of the Impulse Response Via Correlation Techniques

imperfect pulse method, by numerical integration of the transient response to an arbitrary forcing function measured at two locations in the system" [376]. The technique is, experimentally, similar to pulse testing but has been most widely used in "tracer" studies to determine parameters in mixing models for flow systems [376-378].

Computational Techniques and Reliability Estimates

This method involves calculating weighted moments of the experimental data and equating these numeric values to appropriate functions of the Laplace transform of the assumed model, $G(s)$. The n th moment of the normalized experimental response, $C(t)$, can be calculated from:

$$M^n(s) = \int_0^{\infty} \exp(-st) C(t) t^n dt \quad (58)$$

Moments could also be calculated from equation (58) using values of $C(t)$ calculated from the assumed model. However, to avoid having to calculate the time domain solution, use is made of Laplace transform theory to show that equation (58) is defined as the transform of $t^n C(t)$ and that:

$$M^n(s) = (-1)^n \frac{d^n}{ds^n} C(s) \quad (59)$$

It should be noted that if the input forcing function, $C_i(t)$, is a pure impulse then $C_i(s) = 1$ and $C_0(s) = G(s)$. In the more general case the assumed transfer function model is related to the transforms of the system input and output by the following relationships:

$$G(s) = \frac{C_0(s)}{C_i(s)}$$

$$\frac{d^m G'(s)}{ds^m G(s)} = \frac{d^m}{ds^m} \left[\frac{C'(s)}{C(s)} \right] \Big|_i^0 , \quad m = 0, 1, 2, \dots \quad (60)$$

Thus in practice the model parameters are obtained by solving the set of non-linear algebraic equations that results from equations (60). The transform of the assumed model, $G(s)$, is substituted into the left hand side of equations (60) and the values of $C(s)$ and its derivatives which arise in the evaluation of the right hand side are replaced by numeric values calculated from the experimental data using equation (58).

Michelsen and Ostergaard [376] present four methods of calculating the model parameters from the moments and show that the sensitivity to experimental errors in the transient responses can be greatly reduced by proper choice of the s parameter.

Mehta and Shemilt [377] work with moments about the origin (equivalent to setting $s = 0$ in the above equation) and present several examples.

This method is particularly convenient when an appropriate model can be specified, and used, directly in the Laplace transform domain. Parameter evaluation for a model containing p parameters requires calculation of at least p moments. If the experimental data, $C_i(t)$ and $C_0(t)$, are accurate then it is normally advantageous to calculate more than p moments and evaluate the parameters by statistical analysis since this permits evaluation of the validity of the model [376]. The transfer function, $G(s)$, can be inverted to yield the impulse response, $g(t)$, or used in frequency response analysis as discussed in section 7.

Experimental Technique

The input must be a closed pulse and the output must be allowed to return to the steady-state value. Truncating time data or 'drifting' of the reference base can cause serious error since the output tail is weighted heavily, especially for higher moments.

Applications

The method of moments has been applied to the modelling of liquid fluidized systems [377], the evaluation of dispersion coefficients for fluid flow systems [376,379] and model reduction [380].

7. FREQUENCY RESPONSE

The frequency response or frequency domain model forms the basis for the classical design and analysis methods of single-variable, linear control systems. It applies to systems described by equation (49) and is normally presented in the form of Bode or Nyquist diagrams. The frequency response of a system can be calculated from the system transfer function ($G(s)$ in equation (49)) or determined by experimental tests which employ periodic, aperiodic or random signals. It can be shown [381] that if a 'stable' linear system is subjected to a sinusoidal forcing function, $u(t) = u_{\max} \sin(\omega t)$, the output (after the initial transient has died out) has the form $y(t) = y_{\max} \sin(\omega t + \theta)$ and that

$$y_{\max}/u_{\max} = |G(i\omega)| \quad (61)$$

$$\theta = \angle G(i\omega) \quad (62)$$

where $|G(i\omega)|$ and $\angle G(i\omega)$ are obtained by replacing the Laplace variable in the system transfer function, $G(s)$, by $i\omega$ and formally calculating the magnitude and angle of the resulting complex expression [381].

The utility of this representation lies in the classical design and analysis techniques that have been developed for direct use in the frequency domain, pure time delays can be easily handled, experimental and/or theoretical

frequency response plots for components can be readily combined into an overall system model, and the stability of feedback control systems can be determined from the open-loop model without having to invert the transforms or perform extensive calculations.

The normal procedure associated with parameter estimation is to determine the frequency response from experimental tests and then fit the data in the frequency domain in order to obtain a transfer function or differential equation model [382-388]. Chen and Haas [389] review several graphical and computer methods for obtaining transfer functions and include computer programme listings for Levy's method [390]. It should be noted that a 'best' fit in the frequency domain does not necessarily yield a 'best' fit in the time domain. The time-domain least-squares criteria can be transformed analytically, using Parseval's theorem, into an equivalent expression in the frequency domain and offers distinct advantages [382,385, 391,392].

A series of twelve articles by Murrill et al. provide an excellent introduction to this area (e.g. [393]). A bibliography of early applications exists [394].

Describing function techniques [395,396] have been used in an attempt to extend the frequency response approach to non-linear systems.

The frequency response approach can also be extended to multivariable linear systems by using matrices of transfer functions but in practice the manipulation of polynomials in the Laplace operator, s , becomes difficult. Multivariate frequency response based on time series (spectral) analysis is well presented by Jenkins and Watts [385]. They show that, as in the single variable case, spectral analysis and frequency response estimation represent extensions of correlation and multivariate time-domain techniques to the frequency domain.

7.1 Frequency Response Testing

General Discussion

The technique is well documented in the literature [397, 398] and textbooks [381] in the automatic control field.

Computational Techniques and Reliability Estimates

If a pure sine wave is used as a forcing function then the ratio of the amplitudes and the relative phase of the input and output signals, as defined by equations (61) and (62), give one point on a frequency response plot [399]. Since a separate test must be run for each point, the method is time consuming and is better applied to fast responding linear devices, such as instruments, than to industrial processes. The method is excellent for determining the system response at specific frequencies and is relatively insensitive to noise. Signal averaging techniques permit valid observations at very low signal-to-noise ratios.

Non-linearities in the system distort the output sinusoid and destroy the accuracy of the test.

Experimental Technique

Generation of the required input sinusoid is often difficult or impossible. Commercial instruments are available for signal generation and data reduction. Band-pass filters are frequently used to reduce noise and the effect of harmonics of the test signal.

Applications

Reference is made to Pollock and Johnson [397] for their treatment using a small-scale extraction column. Other applications to heat exchange equipment [400-403], a fluidized bed reactor [404], extraction columns [405], a distillation column [406,407], and adsorption column [408], pneumatic lines [409] and a respiratory system [410] are reported.

7.2 Pulse Testing

General Discussion [411-420]

This approach is based on the definition of the system transfer function as the ratio of the transform of the output function divided by the transform of the input function. If a 'closed form' or 'pulse' input disturbance is applied to a linear system and the output function is recorded then application of the Laplace transform and the replacement of s by $i\omega$ yields:

$$G(i\omega) = \frac{y(i\omega)}{u(i\omega)} = \frac{\int_0^\infty y(t) \exp(-i\omega t) dt}{\int_0^\infty u(t) \exp(-i\omega t) dt} \quad (63)$$

Thus if the transforms can be found the frequency response follows directly from equation (63). Since a pulse exhibits a continuous frequency spectrum it is often possible, by proper choice of the input signal, to extract the frequency response over the full range of interest from a single test.

Computational Techniques and Reliability Estimates

Using the Euler relationships equation (63) can be separated into real and imaginary parts:

$$G(i\omega) = \frac{\int_0^\infty y(t) \cos(\omega t) dt - i \int_0^\infty y(t) \sin(\omega t) dt}{\int_0^\infty u(t) \cos(\omega t) dt - i \int_0^\infty u(t) \sin(\omega t) dt} \quad (64)$$

The four integrals in equation (64) must be evaluated for the duration of the input and output pulses [415]. The following numerical techniques have been used: the trapezoidal rule [414], Filon's method [414] and the fast Fourier transform technique [393,421,422]. Errors in the analysis arise due to aliasing [423], round-off errors [424], truncation of time data [418,425], frequency content of the forcing function becoming small [426] and also non-

linearities in the process. Comparisons of the different computational techniques and their accuracy have been made [414,426]. Lees and Dougherty [424] did an extensive amount of work with pulse testing and showed that many of the problems of high-frequency degeneration are due to the failure of the numerical approximation to the Fourier integral to converge and that the upper limit in frequency is $\omega T = 0.1\pi$. They also recommend about ten times as many experimental points than are taken in common practice. In a later article Messa, Luyben and Poehlein [456] indicate that fewer data points can be used if they "adequately" define the pulse.

Experimental Aspects

The effect of various pulse shapes have been studied by several authors [415,418,423,426,427], but many shapes are impractical for industrial process applications. If the input variable can be measured accurately the input pulse may be any shape (but some are better than others) and thus be generated manually. However, the input and output shapes must return to the zero position. Truncating the data can cause problems in processes which exhibit a significant tail [418].

Multiple pulses are used by Pollock and Johnson [397] to increase the limiting frequency. Pulses of different areas (power), but identical shapes, can be used to test system linearity.

Applications

Several authors [175,397,412,428] compare pulse testing with other techniques. Applications include a heat exchanger [423,426,429,430], an electric furnace [175], an extraction column [397,405,414,431], flight control [432], a distillation column [405,428], mass transfer in a fluid flow system [433], a control system [434], a partially mixed stirred tank reactor [435] and a wetted wall column [427].

7.3 Frequency Response Data from Transient Response

General Discussion [397,436]

A step function is a convenient test signal because it is easy to generate and response data are often available from normal operating records. The calculational methods applied in the previous section cannot be used directly since the Fourier transform of a step function is not defined. One solution to this difficulty is to differentiate the input and output functions, apply the definition of the Laplace transform to the derivatives and then integrate by parts to yield:

$$G(s) = \frac{\exp(-sT_2)y(T_2) + s \int_0^{T_2} y(t)\exp(-st)dt}{\exp(-sT_1)u(T_1) + s \int_0^{T_1} u(t)\exp(-st)dt} \quad (65)$$

Replacement of s by $i\omega$ permits calculation of the frequency response.

If it is desired to obtain a time-domain model from experimental step response data then the methods of section 2.5 should be considered instead of finding the frequency response and then curve fitting.

Computational Techniques [397,436] and Reliability Estimates

Applicable techniques include Fourier or Laplace transforms [397] and graphical techniques [437-438].

Strobel [439] and Unbehauen and Schlegel [440] study the effect of errors in the time domain on the frequency response data.

Experimental Technique

A step test is normally used [397]. However, Petrovic [441] considers seven other test signals.

Applications

Applications involving a distillation column [391], and an extraction column [397] are reported. Pollock and Johnson [397] conclude this method is as accurate as pulse testing for their system.

7.4 Frequency Response from Spectral Analysis

General Discussion [385]

The Wiener-Hopf equation was used in section 6.3 to obtain the system impulse response from the auto and cross-correlation functions of the system input and output variables, i.e.

$$\phi_{uy}(t) = \int_{-\infty}^{+\infty} g(\tau) \phi_{uu}(t - \tau) d\tau \quad (54)$$

Application of the Fourier transform to equation (54) yields:

$$\Phi_{uy}(\omega) = G(\omega) \Phi_{uu}(\omega) \quad (66)$$

where

$\Phi_{uu}(\omega)$ = spectral density function calculated by taking the Fourier transform of the cross-correlation function defined by equation (55),

$\Phi_{uu}(\omega)$ = spectral density function calculated by taking the Fourier transform of the autocorrelation function defined by equation (56),

$G(\omega)$ = system frequency response.

The power spectral density functions have physical meaning as a measure of the power content of a signal as a function of frequency. Methods of generating random test signals with a particular power density spectrum have been reported [442]. This technique is of particular value when system response data for 'random' inputs are already available. However, long data records (often several thousand points) are frequently required to produce the desired accuracy.

Computational Technique and Reliability Estimates [385,393,412,443-449]

One computational approach is to evaluate the convolution integrals which define the spectral density functions and then to evaluate $G(\omega)$ from equation (66). This rather complicated data-processing technique tends to be inaccurate unless special techniques such as the use of 'spectral windows' are used to smooth the estimates, remove the effect of output drift and of data truncation [385].

The reader should consult references such as Jenkins and Watts [385] before using these techniques. They discuss the importance of considering the statistical properties of the estimators, the implication of correlation between the various signals, the relative advantages of different calculations approaches and the relationship to familiar least-squares techniques.

The degree of causality (dependence) of an output $y(t)$ on the input $u(t)$ vs. unrelated process noise $n(t)$ can be defined by calculation of a coherence function [385,450]. The effects of the noise can be reduced by proper averaging techniques if replicate runs are available.

Confidence limits for the estimates of the phase and gain at each point can be calculated [385,444,447].

Experimental Technique

The forcing function is normally a random signal. It can be the normal process operating record [316], pseudo-random binary chain code [246] or random telegraph signal [444]. These test signals are easily applied. The test is not sensitive to other disturbances.

Applications

Hutchinson and Shelton [444] apply this scheme to an oil-refinery depropanizer column in an excellent treatment of the method. Comparison of this method with other testing procedures is considered in [175] and [412]. The method has been applied to identification of heat exchangers [451], reactor systems [452-454] and packed towers [455].

8. CONCLUSIONS

It is obvious from this review and previous ones that there are a great many different methods for process identification and parameter estimation and an abundance of literature dealing with their development and application. The author feels that in addition to further work on individual methods there is a need for comparative studies and increased emphasis on applications. Discussion of reliability estimates, relationship to other methods, effects of noise, practical aspects of implementation, etc. would make many presentations more complete, and the use of 'standardized' examples would facilitate direct comparison of methods. This paper is intended as another step in this direction and to assist the reader in selecting a method for his particular area of interest.

CHAPTER THREE

PARAMETER ESTIMATION USING QUASILINEARIZATION

ABSTRACT

A generalized approach to process identification is developed in this chapter. The algorithm, which combines linear programming with quasilinearization, is formulated and many of the practical aspects of its implementation, including computation and convergence, are explored.

Examples are presented to illustrate application of the algorithm to real engineering problems, to demonstrate the incorporation of constraints and to introduce a technique for extending the region of convergence of the algorithm.

1. INTRODUCTION

One of the most common problems in engineering analysis is the determination of parameters in a mathematical model such that the model response satisfactorily reproduces or "best" fits experimental data taken from the physical system of interest.

A convenient representation for the mathematical model of many dynamic systems is the vector differential equation:

$$\dot{\underline{x}}(t) = \underline{f} [\underline{x}(t), \underline{u}(t), \underline{p}(t)] \quad (1)$$

$$\underline{y}(t) = \underline{h} [\underline{x}(t), \underline{u}(t), \underline{w}(t)] \quad (2)$$

where

$\underline{x}(t)$ = state vector ($n \times 1$)

$\underline{u}(t)$ = input or control vector ($m \times 1$)

$\underline{p}(t)$ = unknown parameters vector ($p \times 1$)

$\underline{y}(t)$ = output vector ($r \times 1$)

$\underline{w}(t)$ = measurement noise ($r \times 1$)

The parameter estimation problem is to determine $\underline{p}(t)$ such that the model optimizes a specified objective function such as minimizing the sum of the differences between the model response and the discrete experimental data points. There are many techniques available for the solution of this inverse problem [1] but one of the most general and powerful approaches is to transform the parameter identification problem into a boundary value problem. This transformation can

be made by defining $\underline{z}(t)$ to be the augmented state variable:

$$\underline{z}(t) = \begin{bmatrix} \underline{x}(t) \\ \underline{p}(t) \end{bmatrix} \quad (3)$$

and

$$\dot{\underline{z}}(t) = \begin{bmatrix} \dot{\underline{x}}(t) \\ 0 \end{bmatrix} \quad (4)$$

since for the time invariant model $\underline{p}(t) = \underline{p}$. In terms of the augmented state vector equations (1) and (2) become:

$$\dot{\underline{z}}(t) = \underline{g} [\underline{z}(t), \underline{u}(t)] \quad (5)$$

$$\underline{y}(t) = \underline{h} [\underline{z}(t), \underline{u}(t)] + \underline{w}(t) \quad (6)$$

The parameter estimation problem may now be stated as one of determining part or all of the initial conditions of the state vector such that an index of performance is minimized. The index of performance is usually some function of the residuals which are defined as the difference between observed values and those predicted by equations (5) and (6). Thus a boundary value problem similar to that which arises in optimal control theory must be solved.

There are many computational approaches to this boundary value problem [2], however, one of the most promising is quasilinearization which was selected for this work on that basis as well as the fact that previous work had been done

on quasilinearization as a numerical method in the department [3]. The desire to be able to incorporate as much a priori knowledge of the system as possible into the problem solution as well as the need to alleviate ill conditioning problems led to the use of linear programming in the algorithm presented in this work.

Other authors have used quasilinearization for parameter estimation problems [2,3,4,5,6,7] and developed the theoretical basis for the approach. This work is concerned primarily with the following practical aspects which are required for a useful, generalized algorithm:

- (1) formulation and computational aspects
- (2) use of different linear performance indices
- (3) incorporation of constraints on the parameters and/or state variables
- (4) generating reliability estimates of parameters
- (5) extending the region of convergence of the quasilinearization algorithm.

Four examples are presented to illustrate the application of the quasilinearization plus linear programming algorithm developed in this work and include experimental evaluation of the derived models.

2. FORMULATION AND THEORY OF QUASILINEARIZATION

The quasilinearization approach treats the nonlinear boundary value problem as a series of linear problems which hopefully converge to a feasible solution [3,8].

Expanding the right-hand side of equation (5) in a first order Taylor series the value of the right-hand-side vector at the $(m + 1)^{st}$ iteration may be calculated in terms of the previous iteration:

$$\underline{g}^{(m+1)} = \underline{g}^{(m)} + \underline{J}^{(m)} \left[\underline{z}^{(m+1)} - \underline{z}^{(m)} \right] \quad (7)$$

where the arguments of the functions have been dropped for clarity. The matrix $\underline{J}^{(m)}$ is the Jacobian matrix the elements of which are defined as:

$$J_{ij}^{(m)} = \frac{\partial g_i^{(m)}}{\partial z_j^{(m)}} \quad (8)$$

The linearized version of equation (5) becomes:

$$\dot{\underline{z}}^{(m+1)}(t) = \underline{J}^{(m)} \underline{z}^{(m+1)}(t) + \left[\underline{g}^{(m)} - \underline{J}^{(m)} \underline{z}^{(m)}(t) \right] \quad (9)$$

Application of the principle of superposition [9] leads to the well known solution in terms of the sum of a homogeneous and a particular solution, $\underline{z}_p(t)$.

$$\underline{z}^{(m+1)}(t) = \underline{\varnothing}^{(m+1)}(t)\underline{z}^{(m+1)}(0) + \underline{z}_p^{(m+1)}(t) \quad (10)$$

The matrix $\underline{\varnothing}$ is the fundamental or transition matrix which itself is a solution to an ordinary differential equation with initial conditions $\underline{\varnothing}(0) = \underline{1}$. Since the unknown parameters are included in $\underline{z}(0)$, equations (10) serve as constraint equations during the minimization of the performance index. Conventional least squares is a convenient method for estimating $\underline{z}(0)$ from equation (10) and the trajectory data [3,4,5]. However, this approach is often hindered by ill-conditioned linear equations. Linear programming techniques offer a viable alternative.

Figure 1 is a simplified flowsheet depicting the main modules in the algorithm as set up for computer implementation. Based on an initial guess of the unknown parameters which form all, or part, of the vector $\underline{z}(0)$ the particular solution in equation (10) is generated by standard fourth order Runge Kutta integration. The fundamental matrix $\underline{\varnothing}(t)$ is generated in a like manner. A new parameter vector, $\underline{z}^{(m+1)}(0)$ is chosen by standard linear programming techniques so as to minimize the index of performance which is a linear function of the difference between the model response represented by equation (10) and the experimental data. When the current values of the parameters vector differ by an arbitrarily small factor from the previous values, the

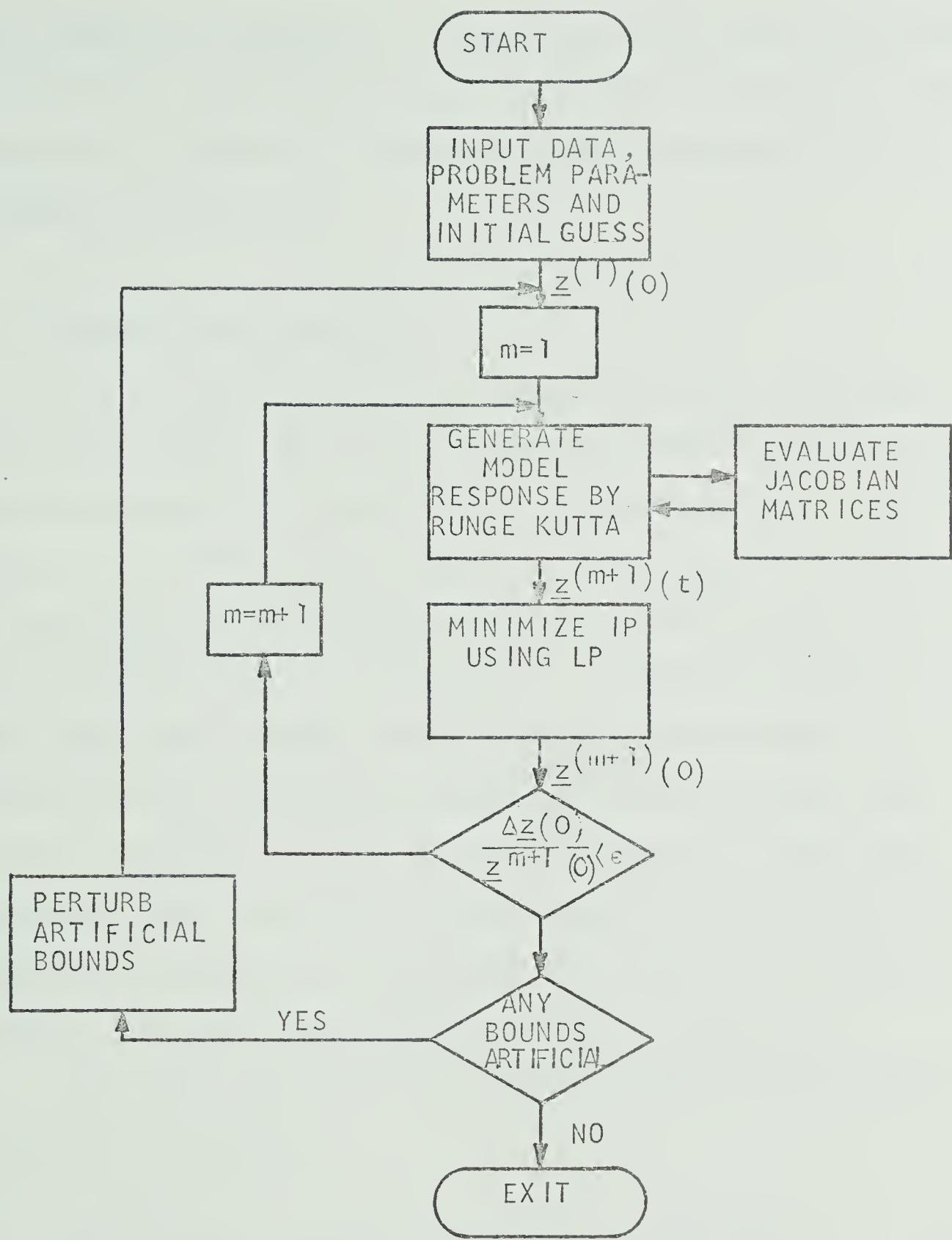


FIGURE 1: Flow Diagram of Parameter Estimation Algorithm

algorithm has converged. If the parameters have not been artificially constrained so as to promote convergence, the solution is complete. The convergence promotion will be discussed subsequently.

3. COMPUTATIONAL ASPFCTS

If the quasilinearization algorithm described above were to be applied directly, a massive computational effort would be required to numerically integrate $(N_{DS} \cdot n + p)^2 + (N_{DS} \cdot n + p)$ differential equations where N_{DS} is the number of data sets and n and p are the dimensions of the state and parameter vectors respectively. Donnelly and Quon [4] took advantage of the structure of the problem which results from N_{DS} independent experiments and the fact that in many problems the initial conditions of all the state variables $\underline{x}(0)$ are known. These simplifications meant the number of differential equations which had to be integrated at each iteration was reduced to $(N_{DS} \cdot n + N_{DS} \cdot n \cdot p)$.

With these modifications equation (10) can be expressed in the following form:

$$\underline{x}_j^{(m+1)}(t) = \underline{G}_{pj}^{(m+1)}(t) \underline{p}^{(m+1)} + \underline{v}_j^{(m+1)}(t) \quad (11)$$

where $\underline{v}_j(t)$ is the particular solution starting with known initial conditions and $\underline{G}_{pj}^{(m+1)}$ is the fundamental matrix associated with the unknown parameters, \underline{p} . The subscript j has been added to indicate multiple data sets.

Example 4 below will demonstrate that with minor adjustments to the problem formulation the algorithm can be applied directly even where some of the initial conditions are not known.

Ramaker et al [5] report that calculation of the change in parameter estimates removes the necessity of generating the particular solution (i.e. only $(N_{DS} \cdot n \cdot p)$ equations need be integrated). These authors also outline means of minimizing core storage requirements at the expense of computer running times.

The greatest potential for improvement in computational time can be achieved in the numerical integration step. The algorithm reported in this work employs a fourth order Runge Kutta procedure. The more sophisticated predictor-corrector methods are more efficient and could be substituted directly. Ramaker et al [5] report successful use of the rectangular integration method in the quasilinearization method.

In order to reduce storage requirements the latest (*i.e.* m^{th}) trajectory was not stored but rather the previous (m) trajectories were regenerated at the $(m+1)^{\text{st}}$ iteration. Generating the previous solution directly from the nonlinear model (equation (5)) as reported by Ramaker et al [5] would have resulted in a considerable saving of computational effort.

The most computational effort is expended in generation of the fundamental matrix, $\underline{\varnothing}$, in equation (10). An alternative method of generating this matrix is by sensitivity methods which requires perturbation of the initial conditions and generation of the final conditions from the nonlinear model. The fundamental matrix can then be calculated from:

$$\Delta \underline{z}^{(m)}(0) = -(\underline{\varnothing}^{-1})^{(m)} \Delta \underline{z}(t_f) \quad (12)$$

As indicated by equation (8) partial derivatives are required in the quasilinearization solution. Analytical expressions were derived in this work; however this is a tedious task for even a problem of modest dimensions. Finite difference techniques are an attractive alternative. Surkan and Wu [10] make reference to a very convenient formula manipulation language which they use to generate partial derivatives in symbolic form.

As indicated in equations (3) and (4) this formulation required the assumption of constant parameters. Lee [11] presents a very simple technique for relaxing this requirement by assuming the functional form of $p(t)$ to be:

$$p(t) = \underline{\theta}(\underline{a}, t) \quad (13)$$

and the constants, \underline{a} , become the constant parameters which must be determined.

4. LINEAR ESTIMATION

The main difficulty with the quasilinearization method arises from the fact that in using the superposition principle a set of linear equations must be solved. The linear equations arise from the minimization of the performance index with equation (10) representing the model trajectory. Ill-conditioning can therefore render the least squares approach useless [12]. Through use of the Chebyshev criterion or the sum-of-absolute-error (SAE) criterion, linear programming techniques can be used and the problems with ill-conditioning are reduced [13]. Several other advantages arise from the use of these criteria in conjunction with linear programming:

- (1) the facility with which hard, soft or target type constraints are incorporated into the problem solution [14]
- (2) larger sets of linear equations can be solved using these techniques [13]
- (3) because more a priori knowledge can be incorporated into the problem solution greater stability is usually ensured
- (4) "better" estimates have been reported from the Chebyshev criterion than least squares [6,7] in certain situations.

However disadvantages of this approach are also evident:

- (1) the estimation is an iterative procedure when linear programming is used [15] whereas the least squares problem has a closed form solution in the form of the well known "normal" equations
- (2) as is the case with least squares the constraint equations must be linear with respect to the parameters
- (3) the linear programming algorithm has a tendency to hunt for an optimum which only improves the solution minutely [16]
- (4) unlike least squares which results in estimates which have many of the desirable statistical properties of an estimator [17] (efficient, unbiased and identical to maximum likelihood estimators for systems with Gaussian noise) the Chebyshev and SAE criteria produce estimates which are only consistent [18].

The least squares formulation has been reported elsewhere [4,12,19] and will not be repeated here. However, the Chebyshev and SAE criteria will be formulated in considerable detail. In the subsequent sections it is assumed that the output vector $\underline{y}(t)$ ($r \times 1$) is simply a subset of the state vector, $\underline{x}(t)$ ($n \times 1$). x_{ijk} will denote value of the i^{th} state variable of the j^{th} data set at time, t_k .

4.1 Chebyshev Criterion

The Chebyshev criterion is simply minimization of the maximum difference between the calculated (from equation (10)) and the observed, $\underline{y}(t)$, values. The maximum deviation, λ , is defined to be:

$$\lambda \geq \left| \frac{x_{ijk} - y_{ijk}}{s_{ijk}} \right| \quad \begin{matrix} i = 1, 2, \dots, r \\ \text{for all } j = 1, 2, \dots, N_{DS} \\ k = 1, 2, \dots, N_j \end{matrix} \quad (14)$$

from which

$$\begin{aligned} x_{ijk} + s_{ijk} \lambda &\geq y_{ijk} & i = 1, 2, \dots, r \\ -x_{ijk} + s_{ijk} \lambda &\geq -y_{ijk} & \text{for all } j = 1, 2, \dots, N_{DS} \\ && k = 1, 2, \dots, N_j \end{aligned} \quad (15)$$

where s_{ijk} is a weighting factor assigned to the i^{th} state variable in the j^{th} data set at time t_k . Substituting equation (11) into equation (15), the following matrix equations can be formed:

$$\begin{aligned} \underline{G}_{pj}(t) \underline{p} + \underline{s}_j(t) \lambda &\geq \underline{y}_j(t) - \underline{v}_j(t) \\ -\underline{G}_{pj}(t) \underline{p} + \underline{s}_j(t) \lambda &\geq -\underline{y}_j(t) + \underline{v}_j(t) \end{aligned} \quad (16)$$

Formulating the linear estimation problem as a linear programming problem, the object is to minimize the linear objective function, λ , subject to the linear constraints formed

from equations (16). If constraints on \underline{p} can be expressed as:

$$\underline{A}_p \underline{p} \geq \underline{c}_p \quad (17)$$

and hard constraints on $\underline{x}(t)$ can be expressed as:

$$\underline{G}'_{pj}(t) \cdot \underline{p} \geq \underline{c}_x(t) - \underline{v}_j(t) \quad (18)$$

the complete LP problem can be summarized by:

$$\text{minimize: } z = \lambda$$

subject to:

$$\left[\begin{array}{c|c} \underline{G}_{pj}(t_k) & \underline{s}_j(t_k) \\ \hline -\underline{G}_{pj}(t_k) & \underline{s}_j(t_k) \\ \hline \underline{G}'_p(t_k) & 0 \\ \hline \underline{A}_p & 0 \end{array} \right] \left[\begin{array}{c} \underline{p} \\ \lambda \end{array} \right] \geq \left[\begin{array}{c} \underline{y}_j(t_k) - \underline{v}_j(t_k) \\ \hline -\underline{y}_j(t_k) + \underline{v}_j(t_k) \\ \hline \underline{c}_x(t_k) - \underline{v}_j(t_k) \\ \hline \underline{c}_p \end{array} \right] \quad (19)$$

where k and j vary over all possible values as per equation (15).

Equation (19) has $(2r(\sum_j N_j) + p + n(\sum_j N_j))$ rows and $(p + 1)$ columns. Since the number of iterations taken to solve a linear programming problem is proportional to the number of rows only, the dual problem to that summarized

in equation (19) results in greater computational efficiency [15]. The number of iterations is dependent only on the number of unknown parameters and is independent of the number of state variables and data points.

Caution must be taken when using this fitting criterion since poor data points can render the estimation useless. However careful examination of the "controlling" data points can often result in the location of data points with gross errors [20].

Note that constraints on the state variables are forced only at sampling instants.

4.2 Sum of the Absolute Errors (SAE)

Another linear criterion can be defined as the sum of the absolute deviations between the model response and the experimental data:

$$z = \sum_{j=1}^{N_{DS}} \sum_{k=1}^{N_j} \sum_{i=1}^r w_{ijk} |x_{ijk} - y_{ijk}| \quad (20)$$

In a form which is more convenient for linear programming techniques:

$$z = \sum_{j=1}^{N_{DS}} \sum_{k=1}^{N_j} \sum_{i=1}^r \epsilon_1_{ijk} - \epsilon_2_{ijk} \quad (21)$$

where

$$\epsilon_1_{ijk} - \epsilon_2_{ijk} = x_{ijk} - y_{ijk} \quad (22)$$

and

$$\epsilon_1_{ijk} \geq 0, \quad \epsilon_2_{ijk} \geq 0$$

The linear programming problem becomes: minimize the objective function, Z , as defined by equation (21) subject to (from equation (11)):

$$G_p(t_k) p + \underline{\epsilon}_j(t_k) - \overline{\epsilon}_j(t_k) = y_j(t_k) - v_j(t_k) \quad (23)$$

for all j and k . Constraints on the state and parameter vector can be appended to equation (23) in a similar manner to that outlined above for equation (19). However, this formulation results in $r(\sum_j N_j)$ rows and $r + 2r(\sum_j N_j)$ columns (disregarding constraints) which indicates the primal solution is more efficient. In this case, therefore, the number of linear programming iterations is dependent upon the number of state variables and data points. Obviously the SAE criterion is less attractive than the Chebyshev criterion from a computational point of view.

5. PREDICTION OF THE RELIABILITY OF PARAMETERS AND ACCURACY OF THE MODEL

A factor often overlooked in the estimation of parameters is the estimate of the reliability of the parameters. The estimates of the validity of the parameters can be useful in the design of subsequent experiments so as to obtain data which facilitate complete and accurate model determination. Therefore, it is not always as important to obtain accurate estimates of the elements in the covariance matrix for the parameters as it is to determine which estimates are in doubt.

The sensitivity matrix, $\underline{G}_{pj}(t)$, required in reliability estimation is inherent in the quasilinearization algorithm. Heineken et al [21] and Seinfeld and Gavalas [19] apply quasilinearization with the reliability analysis developed by Rosenbrock and Storey [22] for the least squares criterion.

A similar analysis is applicable when linear programming techniques are used. In general a linear programming problem may be expressed as:

$$\min: \quad Z = \underline{c}^T \underline{x} \quad (24)$$

$$\text{subject to: } \underline{A} \underline{x} \geq \underline{b} \quad (25)$$

The basis matrix, \underline{B} , determines the basic solution to the linear programming problem:

$$\underline{x}_B = \underline{B}^{-1} \underline{b} \quad (26)$$

where it is implicitly understood that all variables not associated with the columns of \underline{A} appearing in \underline{B} are zero.

Corresponding to any \underline{x}_B , a vector \underline{c}_B is defined, the elements of which are the coefficients in equation (24) associated with the basic variables (elements of \underline{x}_B).

The dual variables of the linear programming problem of equation (25) are derived from:

$$\underline{w}_B = (\underline{B}^{-1})^T \underline{c}_B \quad (27)$$

Neglecting for the moment constraints on the parameters and states, the dual formulation to the linear programming problem of equation (19) becomes:

$$\text{maximize: } Z' = \underline{\delta}^T \underline{w} \quad (28)$$

$$\text{subject to: } \underline{A} \underline{w} \leq \underline{b}$$

where

$$\underline{\delta} = \left[\begin{array}{c} \frac{\underline{y}_j(t_k) - \underline{v}_j(t_k)}{-\underline{y}_j(t_k) + \underline{v}_j(t_k)} \end{array} \right]$$

$$\underline{A} = \left[\begin{array}{cc} \frac{\underline{G}_{pj}^T(t_k) - \underline{G}_{pj}^T(t_k)}{\underline{s}_j^T(t_k) - \underline{s}_j^T(t_k)} \end{array} \right]$$

for all k, j and $\underline{b}^T = [0 \ 0 \ \dots \ 1]$. Since $\underline{y}_j(t)$ is the only vector which is subject to random error, the covariance matrix of the dual variables to the problem of equation (28) is:

$$\underline{C}(\underline{\omega}_B) = (\underline{B}^{-1})^T \underline{V}(\underline{\delta}) (\underline{B}^{-1}) \quad (29)$$

where $\underline{\omega}_B^T = [\underline{p}; \lambda]$ since the dual of the dual is the primal. From the definition of $\underline{\delta}$, $\underline{V}(\underline{\delta})$ is equal to $\underline{V}(\underline{y})$. Usually the covariance matrix of the measured values is not known more accurately than

$$\underline{V}(\underline{y}(t)) = \sigma^2 \underline{I} \quad (30)$$

Equation (29) forms the basis for the reliability estimates derived from the Chebyshev criterion. A similar analysis is applicable for the SAE criterion. Recall that \underline{B}^{-1} is obtained directly from the revised simplex algorithm.

The diagonal elements of $\underline{C}(\underline{\omega}_B)$ are the variance estimates of the corresponding elements of $\underline{\omega}_B$. The off diagonal elements are covariance estimates and they indicate the interaction between parameters. Statistically independent parameters have a covariance of zero.

The variance estimates reported in this work are consistent with those reported by Babbar [23].

6. PROMOTION OF CONVERGENCE

Although quasilinearization exhibits quadratic convergence, its domain of convergence is considerably smaller than other techniques such as gradient methods or invariant imbedding [2]. Consequently these other techniques have to be used as a "starter" for quasilinearization [12]. Ramaker et al incorporate Marquardt's method into the quasilinearization procedure to extend the domain of convergence. Donnelly and Quon [4] proposed an unique scheme whereby the experimental data are perturbed such that the initial trajectories are within a specified maximum deviation. The magnitude of subsequent data perturbations is governed by the effect on the unknown system parameters. If the change in the parameters is deemed too large (or small) the data is moved closer to (farther from) the current trajectories.

A more intuitive approach is presented here. Since linear programming techniques allow constraints on the parameters, the search region can be limited in parameter space by constraints. Then upon convergence the region can be shifted until the solution is no longer contrained by artificial bounds.

Subsequent examples will demonstrate the technique and its effectiveness.

7. RESULTS

The new convergence technique introduced previously is illustrated by application to some typical identification problems. Practical factors with regards to the computation and the evaluation of the fitted model are discussed.

7.1 Modelling a Pilot Plant Evaporator

The parameter estimation techniques were applied to a pilot scale, double effect evaporator which is used for process dynamics and control studies at the University of Alberta. Refer to Appendix A. The principal components of the unit are the two effects.

7.1.1 Derived Model Fitting

Material and energy balances based on appropriate assumptions produce the dynamic model presented in Appendix B, which is composed of five nonlinear differential equations and a set of algebraic equations as presented by Newell and Fisher [24] and similar to those reported by Andre and Ritter [25].

The state variables are the liquid levels, the first effect temperature and first and second effect solution concentrations. Because of large differences in the magnitudes of these state variables, normalized perturbation variables are desirable.

A complete discussion of the development of this model, a comparison with other models, and a comparison with experimental results is available [24,26]. Although actual transportation lags and heat transfer dynamics are known to be small, the model response leads the experimental process response by several minutes. Since an accurate model was required for state driving purposes the nonlinear model was coded for the parameter estimation program. The unknown constants were assumed to be the heat transfer conductances, UA_1 and UA_2 , the heat loss terms, HL_1 , HL_2 , and HL_3 and the steady state holdups in each effect, \bar{W}_1 and \bar{W}_2 . The holdups were included since they are the parameters with the largest effect on the dynamic response and can be adjusted to compensate for the omission of effects, such as tube wall dynamics, from the model. The heat loss terms were not arbitrary in that closure of the initial steady state energy balance had to be forced through the use of constraints. In fact HL_1 was a fixed parameter and HL_2 and HL_3 were related by the linear constraint that their sum was equal to a constant determined from steady state data.

Figure 2 compares the theoretical model response (dashed), the fitted model response (solid) and the process response (symbols) for an equivalent disturbance. This plot shows that the lead exhibited by the theoretical model can be substantially reduced by fitting the model to the process response. The gain of the fitted model can be forced

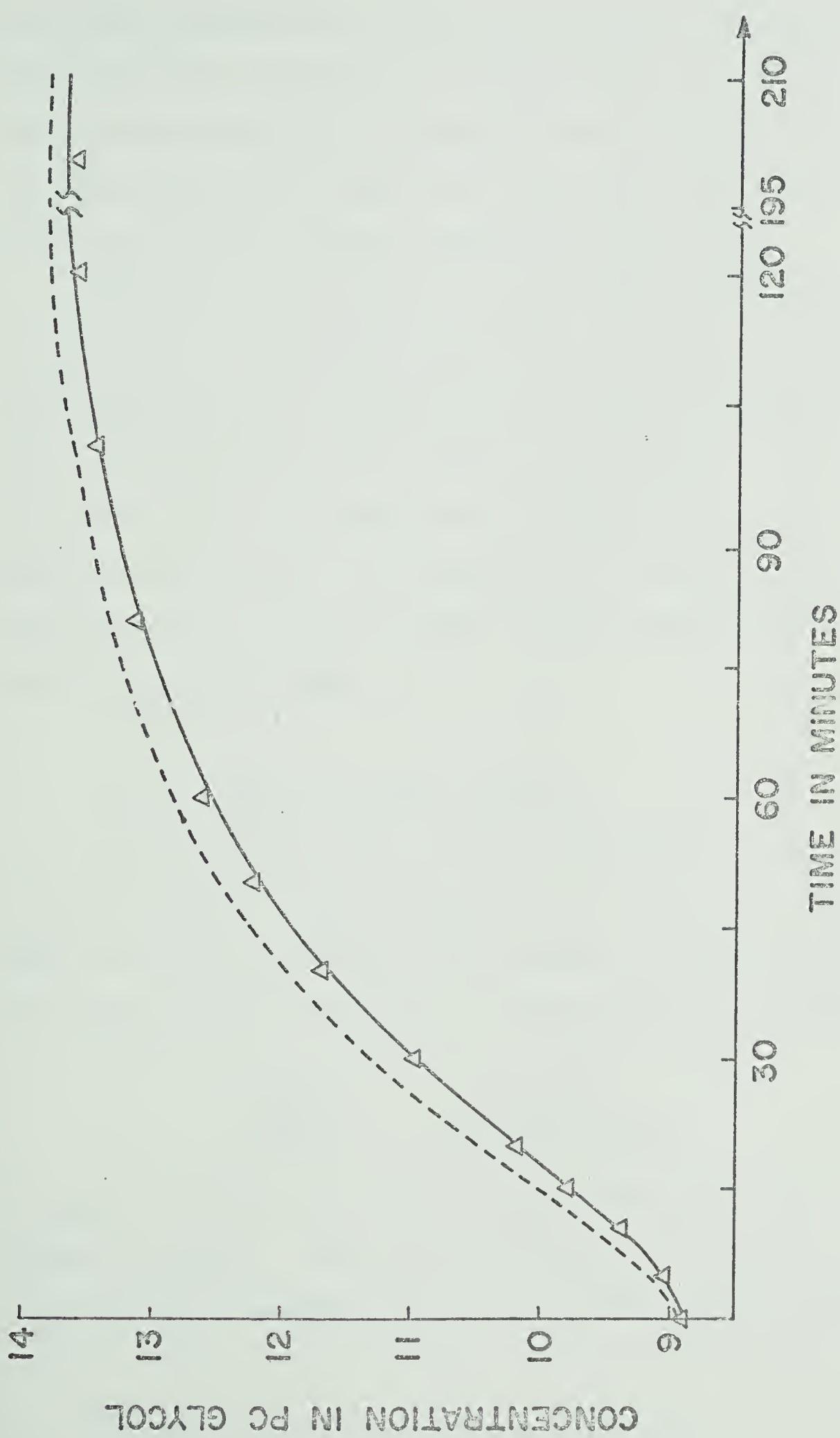


FIGURE 2: Product Concentration Response to 20% Step Steam Flow
— 5NL, — 5LF, Δ experimental.

to closely approximate the experimental by appropriate state variable weighting or constraints on the state variable derivative at the end of the transient. This is demonstrated in Figure 2 by comparing the model trajectories to the process response at large time.

The linearized version of the fitted model produced a much greater improvement over the linearized theoretical model when applied in optimal state driving implementation than is suggested by the relative goodness of fit in Figure 2. This is demonstrated in Chapter 5. This emphasizes that the true adequacy of a model is best evaluated from its performance in the application for which it was obtained.

7.1.2 Empirical Model Fitting

A second order model of the evaporator in the form defined by equation (31) was desired for use in a study of state driving techniques [27] because an analytical expression was available for the time optimal switching times.

$$\frac{c_2(s)}{s(s)} = \frac{K e^{-\tau ds}}{(\tau_1 s + 1)(\tau_2 s + 1)} \quad (31)$$

A typical fit of this model to experimental process response is shown by the solid curves in Figure 3. The assumption of constant gain was not satisfactory for the

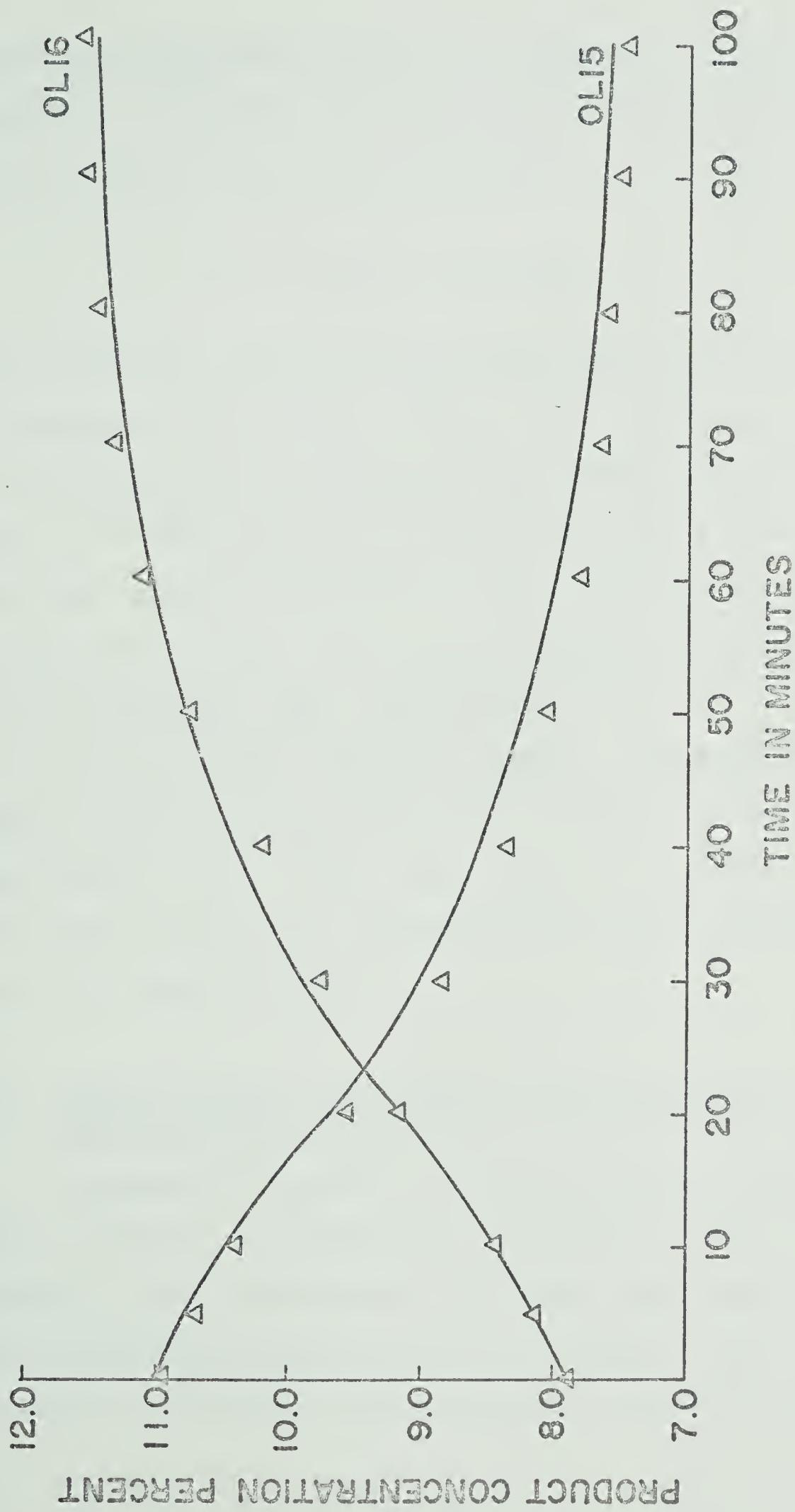


FIGURE 3: Product Concentration Response to Steam Disturbance
— empirical model, Δ experimental.

range of experimental conditions employed. Therefore the following nonlinear expression was derived from the steady state material and energy balances:

$$K = K_L / (1 - K_L \Delta S / C_2) \quad (32)$$

The derivation and evaluation of equation (32) is presented in Appendix 1 for Chapter Three. The time delay, τ_d , can be determined by the parameter estimation algorithm however it is best specified by the user from a priori knowledge and close examination of the experimental results. It was observed that for the experimental response curve of the evaporator many combinations of τ_d and τ_1 and τ_2 produced equivalent "goodness" of fit. However these models performed very differently in the state driving applications [27]. More than a good fit is required emphasizing the need to incorporate a priori knowledge into the identification.

7.2 Identification of a Kinetic Model Using the New Convergence Technique

Frequently a system is encountered where knowledge of the parameters is insufficient to permit a guess close enough to the true solution to obtain convergence. The convergence promotion procedure introduced above is valuable in such an instance. The technique is used to solve a non-

linear reaction kinetics problem solved by Donnelly [28] using quasilinearization and least squares combined with data perturbation. The model can be expressed in the following form:

$$\frac{dx_1}{dt} = -a_1(x_1^2 - ke_1 x_2) - a_2(x_1 - ke_2 x_3) \quad (33)$$

$$\frac{dx_2}{dt} = a_1(x_1^2 - ke_1 x_2) - a_3(x_2 - ke_3 x_3) \quad (34)$$

$$x_3 = 1.0 - x_1 - x_2 \quad (35)$$

where a_1 , a_2 and a_3 are unknown parameters and ke_1 , ke_2 and ke_3 are known equilibrium constants.

Transient data was generated from various initial conditions using the values

$$\underline{a}^T = [2.0 \ 3.5 \ 5.0] \text{ with } \underline{ke}^T = [1.8 \ 3.0 \ 1.0].$$

Donnelly found an initial guess of $\underline{a}^T = [10 \ 10 \ 10]$ would not converge without data perturbation. Using linear programming and quasilinearization the method converged directly without a stepping procedure. This is attributable to the non-negativity constraint inherent in linear programming. The least squares technique on the other hand allows the rate constants to become negative.

The constrained parameter stepping procedure entails assuming an initial parameter vector which is contained in the bounds assigned to each parameter. Change limits must also be assigned to these bounds. A change limit of zero indicates a physical constraint. The change limit is defined as the maximum amount which a bound can be perturbed for the next step.

This approach was used for the initial parameters vector and bounds indicated in Table 1 with an initial change limit of five for all constraints. The results are summarized in Table 1. Figures 4 and 5 illustrate the solution for data set one.

This problem required just over one minute computer time on an IBM 360/67 which is comparable to the time required via least squares solution. The execution times, of course, depend on the initial bounds and change limits which in turn determine the number of steps required.

With reference to Table 1, the maximum number of iterations in Phase I (ie as long as there are artificial constraints) is three since an extremely accurate solution is not necessary. In Phase II the number of iterations may be increased to a maximum value, set in this algorithm to be ten.

The constrained parameter technique, although it is intuitive, may result in an infeasible solution if very poor estimates of the parameters are furnished. The data

TABLE 1
CONSTRAINED PARAMETER STEPPING PROCEDURE

Phase I

Step	Lower Limit	Guess	Upper Limit	Solution Vector	Max Dev.	Itera-tion
1	12	20	25	12		
	12	20	25	12	.371	2
	12	20	25	12		
2	7.0	12	20	7.		
	7.0	12	20	7.	.255	2
	7.0	12	20	7.		
3	2.0	7.0	15.0	2.0790		
	2.0	7.0	15.0	3.2514	.0000776	3*
	2.0	7.0	15.0	4.9154		

Phase II

0.0	2.079	2.0008		
0.0	3.2514	3.4958	.0000625	2
0.0	4.9154	5.00085		

*Maximum Allowable.

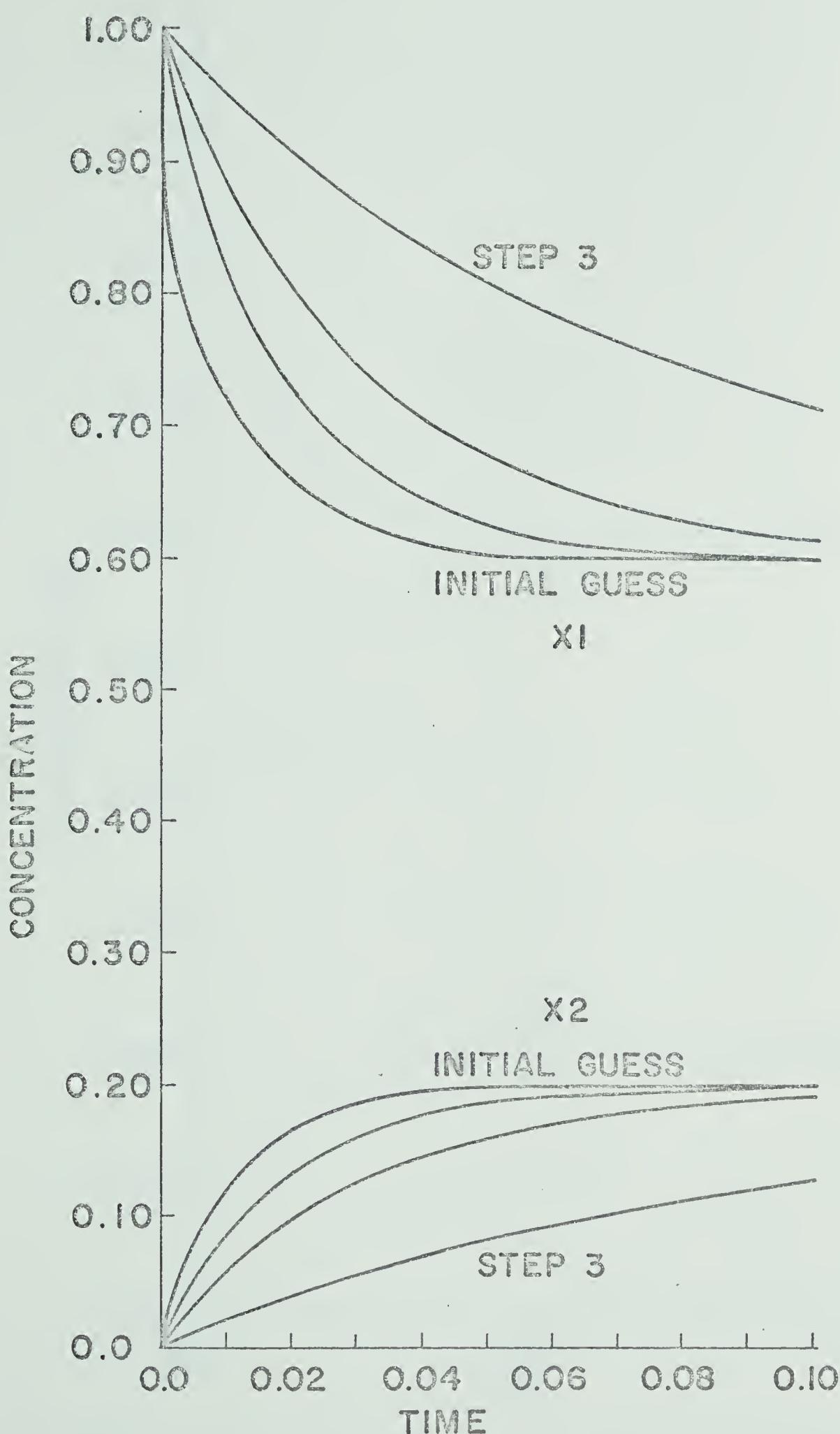


FIGURE 4: Convergence of Nonlinear Kinetics Example Using Constrained Parameter Perturbation (Data Set 1)

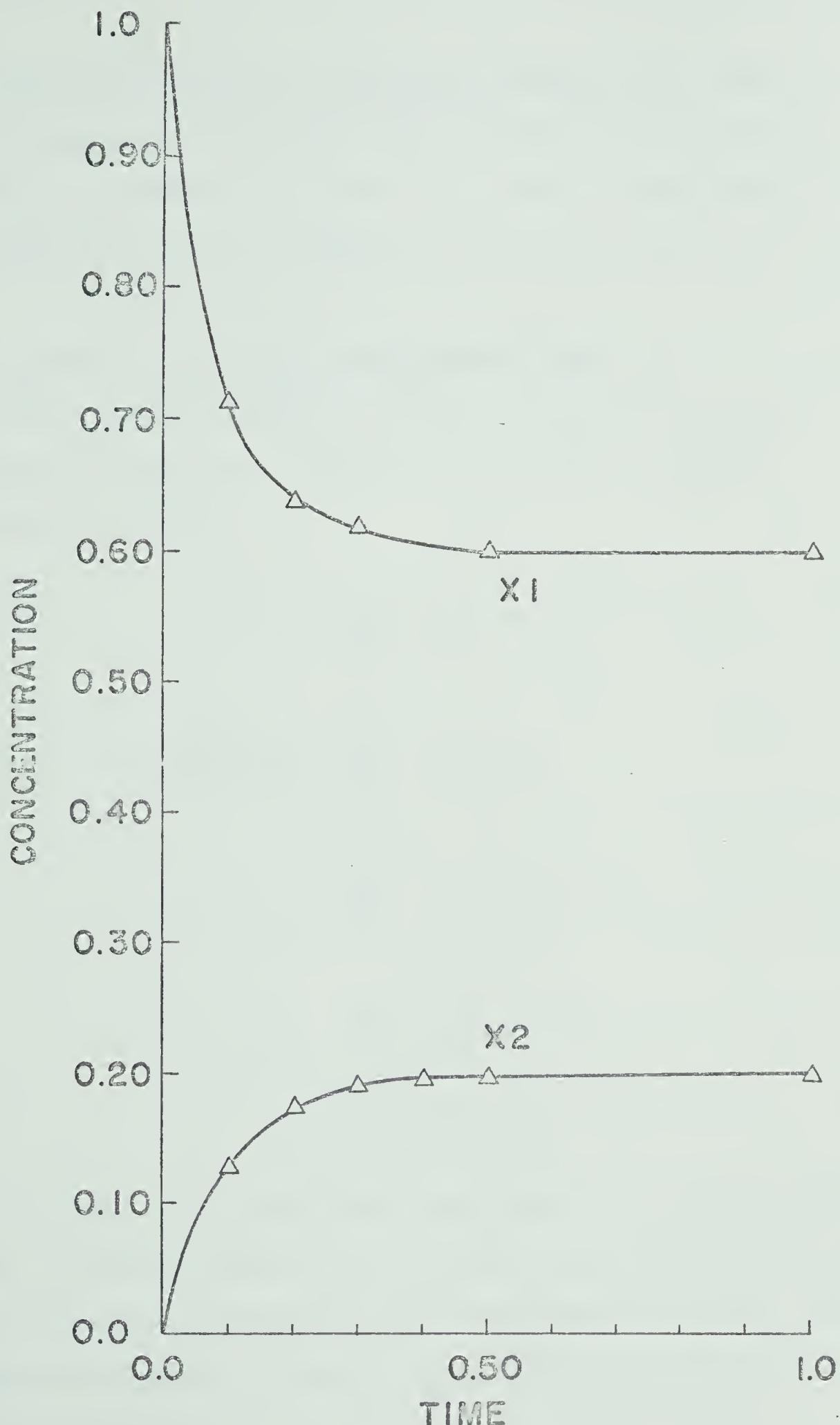
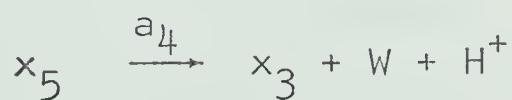
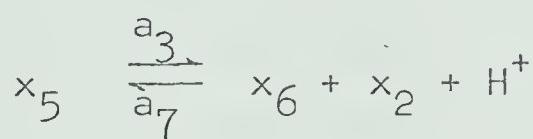
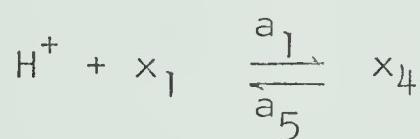


FIGURE 5: Final Solutions of Nonlinear Kinetics Example
(Data Set 1)

perturbation technique proposed by Donnelly and Quon alleviates this problem but the choice of the data perturbation parameters is much less intuitive and the control parameters more difficult to specify a priori.

7.3 Identification of a Complex Reaction

The following mechanism was proposed by Chemcell Limited to describe a reaction of interest to their research personnel:



$$x_6 = \text{Co} - (x_1 + x_3 + x_4 + x_5) \quad (36)$$

Several experiments were performed at constant temperature in a batch reactor. The concentrations of x_1 , x_2 and x_3 were measured throughout the reaction transient. The concentrations H^+ , W and Co were assumed constant for a given experiment.

The following set of ordinary differential equations may be written to describe the above mechanism:

$$\frac{dx_1}{dt} = -a_1 H^+ x_1 + a_5 x_4 \quad (37)$$

$$\frac{dx_2}{dt} = a_2 w x_4 + a_3 x_5 - a_6 x_2 x_5 - a_7 H^+ x_6 x_2 \quad (38)$$

$$\frac{dx_3}{dt} = a_5 x_5 \quad (39)$$

$$\frac{dx_4}{dt} = 0 = a_1 H^+ x_1 - a_5 x_4 - a_2 w x_4 + a_6 x_2 x_5 \quad (40)$$

$$\frac{dx_5}{dt} = 0 = a_2 w x_4 - a_6 x_2 x_5 - a_3 x_5 + a_7 H^+ x_6 x_2 - a_4 x_5 \quad (41)$$

The parameters a_1 through a_7 are unknown and must be determined. The stationary state approximation to equation (40) and (41) reduces the state vector to three components, x_1 , x_2 and x_3 all of which are observed.

Fisher [29] approximated the solution to this problem using analog computer techniques. He concluded that a_2 , a_5 and a_6 could not be determined accurately from the data and therefore were assigned values based on other a priori knowledge of the system. The other constants were then determined by adjusting potentiometer settings until a "good" fit was obtained.

Since the linear programming approach allows constraints, the same approach is possible. Use of a seven parameter model with some values fixed is advantageous since if subsequent experimentation resulted in measurement of intermediates etc, these constraints could be relaxed without having to change the model.

The experimental data has been reported elsewhere [28,29] and will not be repeated here. The constrained parameter stepping procedure discussed in the previous example proved effective in the solution of this problem. The results of the identification procedures are presented in Table 2 for the analog and digital techniques.

Except for parameter a_1 and to a lesser degree a_7 , the parameters could not be estimated accurately from the data. This is a direct result of the fact that the reaction intermediates are not measured and that the initial conditions are all on the same variable. However as indicated by Figure 5, these constants do provide an accurate representation of these experimental data.

Donnelly [28] was unable to work with the full seven constant model. However he was able to solve a reduced model which had only four constants in three differential equations. The model was derived from a simplified mechanistic model.

TABLE 2
SEVEN CONSTANT REACTION MODEL IDENTIFICATION

Constants	Analog	Initial	Digital		95% Confidence Limits
			Step 1	Step 2	
a_1	0.64	0.6120	0.6118	0.6122	\pm 0.00328
a_2	1.70	1.7000	1.7000	1.7000	fixed
a_3	2.35	3.000	2.5000	1.0340	\pm 8.60
a_4	0.35	0.4570	0.3826	1.5896	\pm 1.32
a_5	2.00	2.0000	2.0000	2.0000	fixed
a_6	1.00	1.0000	1.0000	1.0000	fixed
a_7	1.05	0.9752	0.9670	0.9649	\pm 0.0495
Sum of Squares	0.000363	--	--	0.0000953	--
Maximum Deviation	--			0.00157	\pm 0.000102

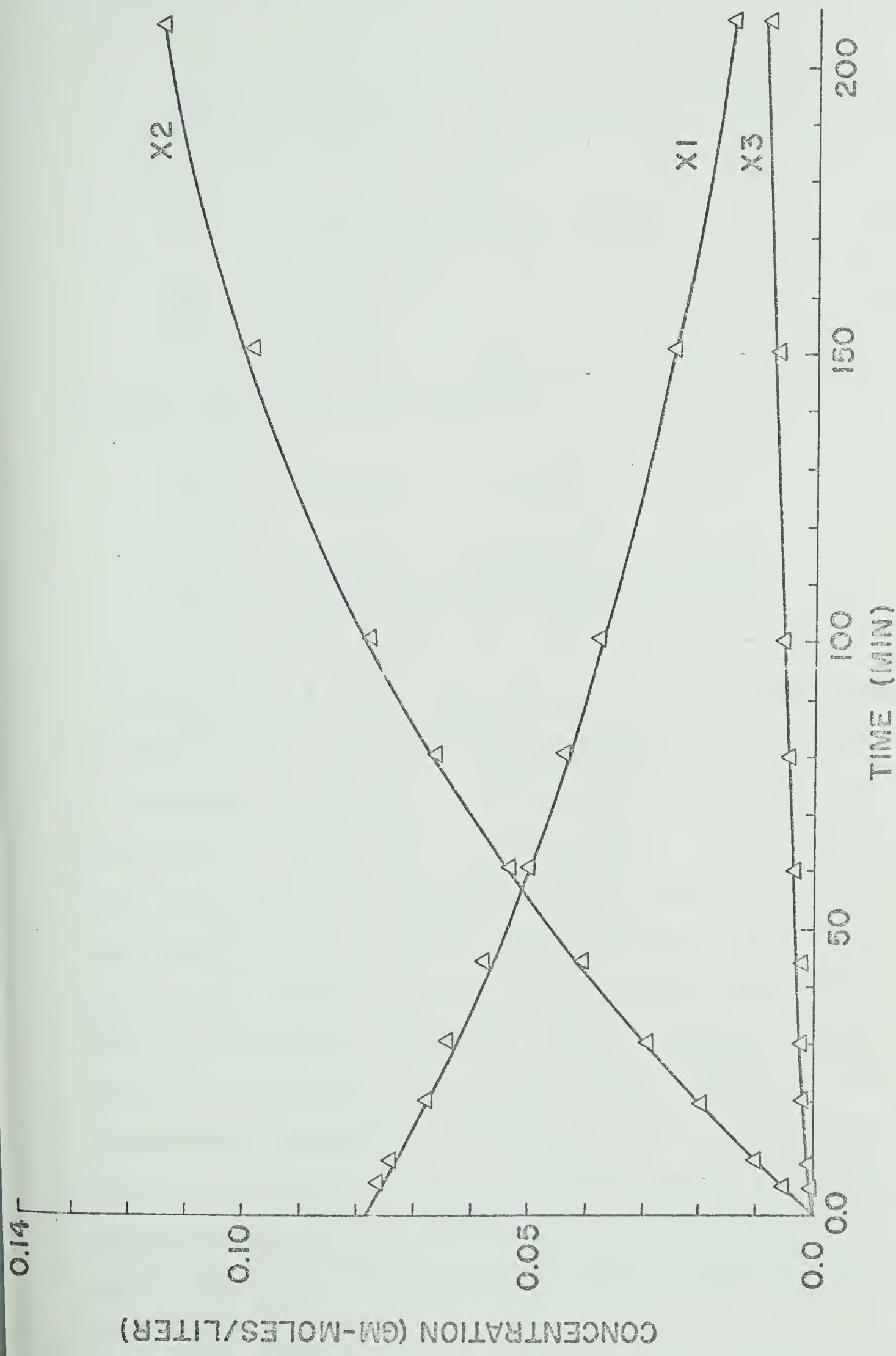


FIGURE 6: Solution to Chemcell Problem (80°C) (Data Set 1)

$$\frac{dx_1}{dt} = -a_1 H^+ w x_1 \quad (42)$$

$$\frac{dx_2}{dt} = a_2 x_4 - a_5 H^+ x_2 x_6 + a_1 H^+ w x_1 \quad (43)$$

$$\frac{dx_3}{dt} = a_3 x_4 \quad (44)$$

and the algebraic relationships

$$x_6 = C_o - (x_1 + x_3 + x_4) \quad (45)$$

$$x_4 = \frac{a_1 x_1 H^+ w + a_1 H^+ x_2 (C_o - x_1 - x_2)}{a_2 + a_3 + a_5 H^+ x_2}$$

Application of the Chebyshev criterion to this problem yielded results equivalent to those obtained by Donnelly as indicated in Table 3. The covariance matrix for the parameters is presented in Table 3 also. It is assumed that the errors and the parameters are normally distributed. The diagonal elements of the matrix are the variances of the parameters. These can readily be converted into confidence limits as was done in Table 2. The off diagonal elements are the covariances. This statistic is a measure of the statistical interaction between constants. The Pearson correlation coefficient [17] is often used as a standard in determining statistical dependence between random variables. Zero indicates no interaction and unity indicates complete interaction.

TABLE 3
 COMPARISON OF LEAST SQUARES AND CHEBYSHEV SOLUTIONS TO
 THE FOUR CONSTANT REACTION MODEL IDENTIFICATION

	a_1	a_2	a_3	a_5	Max Dev	Sum of Squares
Least Squares [28]	0.0106	0.183	0.025	1.37	---	0.000072
Chebyshev	0.01062	0.06173	0.008098	1.7841	0.00153	0.0000854
Co-variance Matrix ($\times 10^8$)	a_1 0.258	a_2 -129.5	a_3 -14.32	a_5 -14.32	-531.01	
(Chebyshev Solution)	a_1 0.01	a_2 -129.5	a_3 -14.32	a_5 -531.01	238,195.	24391.6
					1565959.2	

These variances may be used to determine subsequent experimental approaches or to determine the reliability of the model.

7.4 Identification with Unknown Initial Conditions

As indicated above the number of equations involved in the quasilinearization method is substantially reduced by assuming the initial conditions are known.

This requirement can be relaxed by a simple transformation of variables to perturbation variables. If a system is represented by equation (1) where $\underline{x}(0) = \underline{x}_0$ is not well defined then let $\underline{x}' = \underline{x} - \underline{x}_0$ and the model becomes

$$\begin{aligned}\dot{\underline{x}'}(t) &= f(\underline{x}'(t) + \underline{x}_0, \underline{u}(t), p) \\ \dot{p} &= 0 \\ \dot{\underline{x}}_0 &= 0\end{aligned}\tag{47}$$

where $\underline{x}'(0) = 0$

However there is a loss of accuracy involved in this approach since

$$\underline{V}(\underline{x}') = \underline{V}(\underline{x}) + V(\underline{x}_0)\tag{48}$$

The technique will be illustrated by a simple example presented by Bellman et al [3,6] who solved the problem by

quasilinearization both in conjunction with least squares and linear programming.

The nonlinear second order Van der Pol equation is the system model:

$$\ddot{x} + \lambda(x^2 - 1) \dot{x} + x = 0 \quad (49)$$

where λ is to be estimated from the following experimental observations

$$x(4.0) = -1.80843$$

$$x(6.0) = -1.63385$$

$$x(8.0) = -1.40456$$

In state variable notation equation (49) becomes:

$$\dot{x} = u$$

$$\dot{u} = -\lambda(x^2 - 1)u - x \quad (50)$$

$$\dot{\lambda} = 0$$

where $u = \dot{x}$ and $x = x$. However, since the initial condition, $u(4.0)$, is not measured a new set of state variables is defined such that:

$$\dot{x}_1 = x$$

$$\dot{x}_2 = u - u(4.0) \quad (51)$$

Then λ and $u(4.0)$ can be estimated since:

$$\begin{aligned}
 \dot{x}_1 &= x_2 + u(4.0) \\
 \dot{x}_2 &= -\lambda(x_1^2 - 1)(x_2 + u(4.0)) - x_1 \quad (52) \\
 \dot{\lambda} &= 0 \\
 \dot{u}(4.0) &= 0
 \end{aligned}$$

where $x_1(4.0)$ and $x_2(4.0)$ are known.

Equations (52) are now in a form compatible with the quasilinear identification algorithm employing either least squares or linear programming. The numerical results are summarized in Table 4 for the least squares algorithm.

8. CONCLUSIONS

Quasilinearization in conjunction with linear programming was demonstrated to be an effective general numerical method for the nonlinear boundary value problem arising in parameter estimation.

Several linear performance indices are compatible with linear programming in the context of the algorithm.

A new, intuitive technique for promoting convergence was successfully tested on several nontrivial problems.

Reliability estimates for the parameters are readily generated using the algorithm presented in this paper.

The algorithm allows the incorporation of a priori knowledge of the system in the form of state variable weighting, parameter and state constraints and state variable normalization.

TABLE 4
VAN DER POL PROBLEM RESULTS

Iteration	λ	$u(4.0)$
0	7.0	0.08
1	7.93266	- 0.495475
2	9.91558	0.0527966
3	10.0007	0.0787886
4	10.0004	0.0791647
5	10.0003	0.0790561
final value	10.0004	0.0791116
true value	10.0000	0.079366909

CHAPTER FOUR
COMPUTER CONTROL USING OPTIMAL STATE-
DRIVING TECHNIQUES

ABSTRACT

This paper deals with the determination of an optimal means of driving a multivariable process from one state to another subject to constraints on the control and state variables. The dynamic optimization is based on a linear programming formulation utilizing a process model in the standard state-space form and a minimum time performance criterion. The discrete time series of values produced for each control variable are then applied to the process in an open-loop mode to drive the process to the desired operating state. Results from simulation and experimental studies on a pilot plant scale double effect evaporator operating under computer control are used to illustrate the improvement in performance and some of the factors that arise in practical applications.

1. INTRODUCTION

During the last decade a great many theoretical and simulation studies have demonstrated the potential benefits of optimal multivariable control. Over the same time period a large number of industrial plants have installed real-time process control computers and hence have the hardware capability of implementing optimal control techniques. However, to date, there have been few industrial applications.

The purpose of this paper is to describe the application at the University of Alberta, of optimal state-driving techniques to a pilot plant evaporator controlled by an IBM 1800 computer.

State-driving techniques are a good choice for initial applications in optimal control because:

- (1) every process, even if it is only during start-up and shutdown, is subjected to preplanned changes in operating conditions
- (2) the "bang-bang" control that results from the time optimal control formulation can be implemented, progressively, in any desired number of steps from the familiar "set the inputs to the values applicable at the desired steady state" to the actual optimal procedure

- (3) provided the number of manipulated variables is not excessive the optimal bang-bang sequence can be implemented by the process operators using the "manual" mode of conventional instrumentation
- (4) with the method proposed herein there is no severe limit on the dimensionality of the problem and the optimal control calculations can be done off-line using any standard linear programming system, such as IBM's MPS package.

If a process can be accurately represented by a linear, time-invariant model then techniques for unconstrained optimal control can be applied directly. However in most practical applications the process is non-linear and a satisfactory model cannot be derived on a purely theoretical basis. Therefore, this study compares the results obtained using both theoretical and empirical models of different complexity. It also demonstrates the use of constraints on both the control and state variables.

The following sections include a brief literature survey, a description of the problem formulation and a discussion of the results of simulated and experimental studies.

2. LITERATURE REVIEW

Any optimal control procedure requires careful definition of the criteria. The "time optimal" or "minimum response time" criterion is used in this work because it is particularly convenient for analysis and in most instances closely approximates the actual economic criteria. However since linear programming is used to solve the optimal control problem then ITAE, IAE, minimax and minimum rise time (for a specified settleout time and maximum overshoot) can also be employed as objective functions as will be demonstrated in Chapter 5.

Latour, Koppel and Coughanowr [1] present analytical expressions for the optimal switching times for any over-damped single input, single output system that can be adequately represented by a second order transfer function (with or without a pure time delay). Use of this method resulted in significantly better performance than that obtained using a well tuned PID controller and the improvement increased with the magnitude of the change. However, more sophisticated methods are required for multivariable applications. The two most popular approaches of determining the time optimal policy have been dynamic programming and Pontryagin's maximum principle [2]. These methods produce excellent results but often run into numerical and/or dimensionality problems when they are applied to real systems. Zadeh and Whalen [3] showed that the time optimal

and fuel optimal control problems could be reduced to linear programming problems for linear, discrete time-invariant systems and Bondarenko and Filimonov [4] present numerical results based on these two criteria. This linear programming formulation offers the advantages of greater numerical stability and the ability to handle large multivariable systems with constraints on the control and/or state variables.

Lesser and Lapidus [5] use the linear programming formulation to determine the time optimal control of an absorber described by a sixth order state difference equation. Inlet concentrations were used as the control variables in order to linearize the model and were constrained to keep the solution in a feasible region.

Lack and Enns [6] use a minimax objective function and compute the optimal control for a model of a nuclear reactor with twenty-one state variables. Sakawa and Hayashi [7] extend the discrete linear programming formulation to obtain approximate solutions for continuous systems. Torn [8] points out that the linear programming solution might not be unique under all conditions. However this approach appears to be valid for the majority of chemical engineering problems.

3. DESCRIPTION OF EQUIPMENT

The optimal state driving control techniques described in this paper were applied to a pilot plant size, double effect evaporator at the University of Alberta. Appendix A contains the equipment details and a brief description of the IBM 1800 control computer. The direct digital control (DDC) monitor was used to operate transmitters and final control elements for the cases reported herein. The three master loops were placed on manual and the control action was implemented by manually changing the setpoints of the three slave loops. Refer to Figure 1.

4. PROCESS MODELLING AND IDENTIFICATION

Before any optimal control calculations can be carried out it is necessary to develop a suitable mathematical model. The models used in this study fall into two categories: those derived by fitting an assumed model form to the actual process response and those based on a theoretical analysis of the evaporator.

For modelling purposes the principal components of the evaporator system are the two effects. A mass balance, component balance and heat balance on each effect yields six first order differential equations. However, the pressure (vacuum) in the second effect is closely controlled and hence the energy accumulation in the second effect can

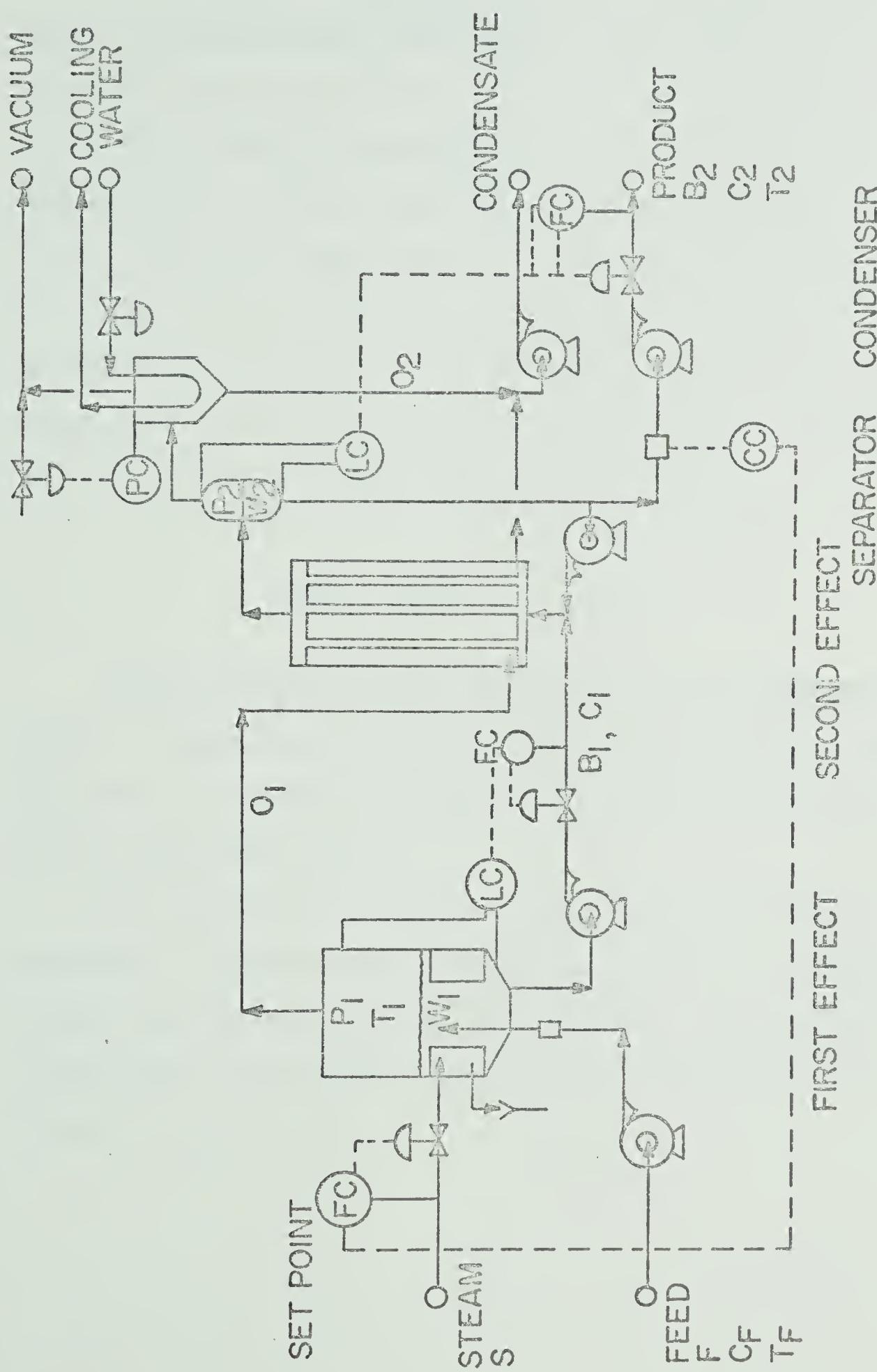


FIGURE 1: Schematic Diagrams of Double Effect Evaporator

be neglected. Similarly the dynamic behaviour of the two steam chests and the inter-effect vapor space can be neglected so that the dynamic model is composed of five non-linear differential equations and a set of algebraic equations similar to those reported by Andre and Ritter [9]. This non-linear model can then be linearized by the introduction of perturbation variables and numerical values calculated for all the coefficients. The result expressed in the standard state variable form, equation (1), is given as linear model 5L1 in Appendix B.

$$\dot{x}(t) = Ax(t) + Bu(t) \quad (1)$$

A more complete discussion of the development of this model, a comparison with other models and a comparison of the model responses with experimental data from the evaporator is available [10].

For state driving purposes the most important state variable is the concentration, C_2 , and this is normally controlled by manipulating the steam, S . It can be shown [10] that by neglecting interactions the transfer function relating C_2 and S is:

$$\frac{C_2(s)}{S(s)} = \frac{K_p(\tau_3 s + 1)}{(\tau_1 s + 1)(\tau_2 s + 1)} \approx \frac{K_p}{(\tau_4 s + 1)} \quad (2)$$

Since analytical methods exist in the literature for second order models it was desired to obtain a model in the following form:

$$\frac{C_2(s)}{S(s)} = \frac{K_p \exp(-\tau_d s)}{(\tau_1 s + 1)(\tau_2 s + 1)} \quad (3)$$

The time constants and gain coefficients in the above two models were determined by means of a parameter estimation method employing quasilinearization and linear programming as discussed in Chapter Three.

Previous experience showed that these simple models gave a reasonable approximation to the process dynamics but due to nonlinearities in the process did not give accurate steady state values for open loop changes of greater than about five percent. Therefore the following gain expression was developed based on a simplification of the non-linear, steady state material and energy balance equations:

$$K_p = KL \left(1 + \frac{\Delta C_2}{C_2} \right) \quad (4)$$

or

$$K_p = \frac{KL}{(1 - KL \frac{\Delta S}{C_2})}$$

This gain expression was particularly valuable in estimating the value of the control variable (steam) to be used at the end of the optimal state driving procedure. The derivation and performance evaluation is presented in Chapter Three.

5. FORMULATION OF THE OPTIMAL CONTROL PROBLEM

For an n^{th} order linear, time invariant, continuous model with real eigenvalues, Athans and Falb (p402[1]) show that the total number of switches in each of the control variables must be less than or equal to $(n - 1)$. (Changes in the control variables that are smaller in magnitude than the difference between the upper and lower constraints are not counted).

Latour et al [1] have shown that for a system described by equation (3) the time optimal control trajectory is of the classic "bang-bang" nature: i.e. at time t_0 , $u(t)$ is set equal to the upper constraint value U_U ; at time t_1 , $u(t)$ is set to the lower constraint value U_L ; and at time t_2 , $u(t)$ is set to the new steady state value. A trajectory of this type is shown in Figure 4. The following implicit expression was derived [1] for time, t_1 .

$$\left[\frac{K_p(U_U - U_L) - r_o - U_L K_p}{(K_p U_U - r)} \exp(-t_1/\tau_2) \right]^{\tau_2/\tau_1} = \frac{K_p(U_U - U_L) - (r_o - U_L K_p) \exp(-t_1/\tau_1)}{(K_p U_U - r)} \quad (5)$$

where: $r < r_o$, $\tau_2 < \tau_1$, $c_2(0) = 0$, $c_2(0) = r_o$.

When required for this work, equation (5) was solved for t_1 using the golden section univariate, direct search algorithm (see Case 2).

The final switch time, t_2 , is calculated from the following explicit equation: [1]

$$t_2 = \tau_1 \ln \left[\frac{r_o - K_p U_L - K_p(U_U - U_L) \exp(t_2/\tau_1)}{r - K_p U_U} \right] \quad (6)$$

For a first order process such as that defined by equation (2) there is only one switching time and it can be calculated from:

$$t_1 = \tau_1 \ln \left[\frac{r_o - K_p U_L}{r - K_p U_L} \right] \quad (7)$$

In all of the above equations if ($r > r_o$) then U_U and U_L must be interchanged. Also if the pure time delay in equation (3) is not zero then the effect of the switches will not be observed for τ_d units of time and in fact the new state will not be attained until $t_2 + \tau_d$ units of time.

If a multi-variable process can be adequately described by the following linear, time-invariant, state-space model:

$$\dot{\underline{x}}(t) = \underline{A} \underline{x}(t) + \underline{B} \underline{u}(t) \quad (8)$$

then the optimal control problem becomes that of determining the trajectories of the control variables, \underline{u} , to drive the system from its initial state, \underline{x}_0 , to the desired final state, \underline{x}_d , while minimizing a particular objective function such as process response time. If the output variables are a linear function of the state only (i.e. $\underline{Y} = \underline{C}\underline{x}$) then the problem can also be stated in terms of \underline{Y} .

The discrete form of the analytical solution to equation (8) can be written [12] as:

$$\underline{x}(k+1) = \underline{\phi} \underline{x}(k) + \underline{\Delta} \underline{u}(k) \quad (9)$$

Repeated use of equation (9) to calculate the state at each time interval yields:

$$\begin{aligned} \underline{x}(1) &= \underline{\phi} \underline{x}(0) + \underline{\Delta} \underline{u}(0) \\ \underline{x}(2) &= \underline{\phi}^2 \underline{x}(0) + \underline{\phi} \underline{\Delta} \underline{u}(0) + \underline{\Delta} \underline{u}(1) \\ &\vdots &&\vdots \\ &\vdots &&\vdots \\ &\vdots &&\vdots \\ \underline{x}(N) &= \underline{\phi}^N \underline{x}(0) + \underline{\phi}^{N-1} \underline{\Delta} \underline{u}(0) + \dots + \underline{\Delta} \underline{u}(N-1) \end{aligned} \quad (10)$$

The computational problem is then to determine the minimum number, N , of control intervals; i.e. the minimum time, required to drive the system to the desired state subject to constraints on the control and/or state variables. To solve this problem a variable λ is defined as

$$\lambda \geq |x_i(N) - x_{di}| \quad \text{for all } i = 1, 2, \dots, n \quad (11)$$

Or in a form more convenient for linear programming.

$$x_i(N) + \lambda \geq x_{di} \quad i = 1, 2, \dots, n \quad (12)$$

$$x_i(N) - \lambda \leq x_{di}$$

In matrix notation, incorporating the expression from equation (10) and defining a vector e_i of weighting factors to be assigned to the state variables, results in equation (13). The solution is an iterative one: a value for the number of sampling intervals, N , is assumed and the linear programming algorithm is used to find the discrete values of the control vector $u(k)$ $k = 1, 2, \dots, N$ that will drive λ to zero. If the solution is successful a smaller value of N is assumed and the procedure repeated until the minimum value of N that will keep λ within the desired limits ($\lambda \approx 0$) is obtained.

Constraints on the state variables at the sampling points are incorporated into the formulation via equation (10). In the most general case these constraints can be

time varying. If each state variable is constrained at each sample time by upper, $\underline{x}_{u,k}$, and lower, $\underline{x}_{L,k}$, limits then the formulation is as shown in equation (14). This represents a linear programming problem with $2(n + Nn)$ rows in $(Nm + 1)$ variables. If the number of rows exceeds the number of variables, then the dual linear programming problem is computationally more efficient [13]. It is apparent from a comparison of equations (13) and (14) that state variable constraints rapidly increase the dimension of the problem. Control variable constraints can be incorporated without increasing the size of the problem [15].

The following sequence of steps was incorporated into a program for an IBM 360/67 computer to generate the control and state variable trajectories:

- (1) Linearize the fifth order non-linear model about the desired steady state
- (2) generate $\underline{\phi}$ and $\underline{\Delta}$ the state difference equation coefficient matrices [14]

$$\begin{bmatrix} \underline{\phi}^{N-1} & \underline{\phi}^{N-2} & \cdots & \Delta & e_N \\ \underline{\phi}^{N-1} & \underline{\phi}^{N-2} & \cdots & \Delta & -e_N \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N-1} \\ \lambda \end{bmatrix} \geq \begin{bmatrix} \underline{x}_d - \underline{\phi}^N \underline{x}_o \\ \underline{x}_d - \underline{\phi}^N \underline{x}_o \end{bmatrix}$$

Equation (13)

$$\begin{bmatrix} \underline{\phi}^{N-1} & \underline{\phi}^{N-2} & \cdots & \Delta & e_N \\ \underline{\phi}^{N-1} & \underline{\phi}^{N-2} & \cdots & \Delta & -e_N \\ \Delta & \underline{o} & \cdots & \underline{o} & \underline{o} \\ \underline{\phi} & \Delta & \Delta & \cdots & \underline{o} & \underline{o} \\ \vdots & & & & & \\ \vdots & & & & & \\ \vdots & & & & & \\ \underline{\phi}^{N-1} & \underline{\phi}^{N-2} & \cdots & \Delta & \underline{o} \\ \Delta & \underline{o} & \cdots & \underline{o} & \underline{o} \\ \underline{\phi} & \Delta & \Delta & \cdots & \underline{o} & \underline{o} \\ \vdots & & & & & \\ \vdots & & & & & \\ \vdots & & & & & \\ \underline{\phi}^{N-1} & \underline{\phi}^{N-2} & \cdots & \Delta & \underline{o} \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N-1} \\ \lambda \end{bmatrix} \geq \begin{bmatrix} \underline{x}_d - \underline{\phi}^N \underline{x}_o \\ \underline{x}_d - \underline{\phi}^N \underline{x}_o \\ \underline{x}_{u_1} - \underline{\phi}^N \underline{x}_o \\ \underline{x}_{u_2} - \underline{\phi}^N \underline{x}_o \\ \vdots \\ \vdots \\ \vdots \\ \underline{x}_{u_N} - \underline{\phi}^N \underline{x}_o \\ \underline{x}_{L_1} - \underline{\phi}^N \underline{x}_o \\ \underline{x}_{L_2} - \underline{\phi}^N \underline{x}_o \\ \vdots \\ \vdots \\ \vdots \\ \underline{x}_{L_N} - \underline{\phi}^N \underline{x}_o \end{bmatrix}$$

Equation (14)

- (3) formulate the linear programming problem as per equation (14) and store it on the disk in the proper format for use by the MPS/360 program
- (4) solve the problem using MPS/360 to get $\underline{u}(k)$ [15]
- (5) generate the state variable trajectories by applying $\underline{u}(k)$ to the process model.

A typical running time for this problem with 5 state variables, 3 control variables, 40 sampling intervals and constraints on the state and control variables was about one minute.

6. DISCUSSION OF RESULTS*

The results of the experimental and simulation studies are presented as a series of five cases ranging from the simplest single-input single-output approach, to multivariable applications based on a fifth order evaporator model with state and control variable constraints.

Figure 2 compares the response of the nonlinear evaporator model when subjected to:

- (a) an open-loop change in steam flow;
- (b) a closed-loop change in setpoint (P and I feedback controller from C_2 to S tuned for regulatory control);

*Refer to Appendix C for additional run documentation

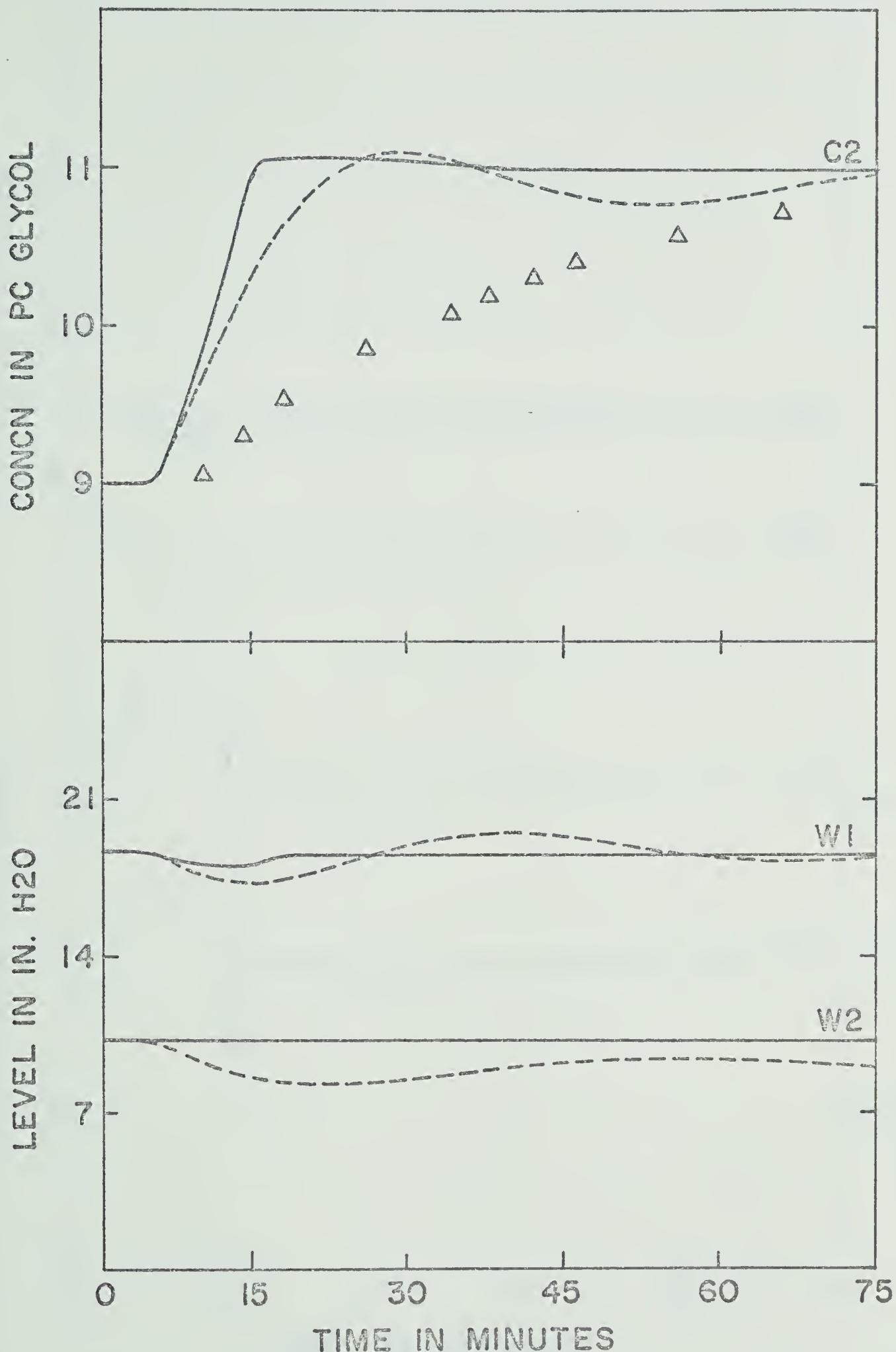


FIGURE 2a: Simulated Responses of Concentration and Liquid Levels Under Optimal, Closed-Loop and Open-Loop Control

— optimal, --- closed-loop, △△△ open-loop

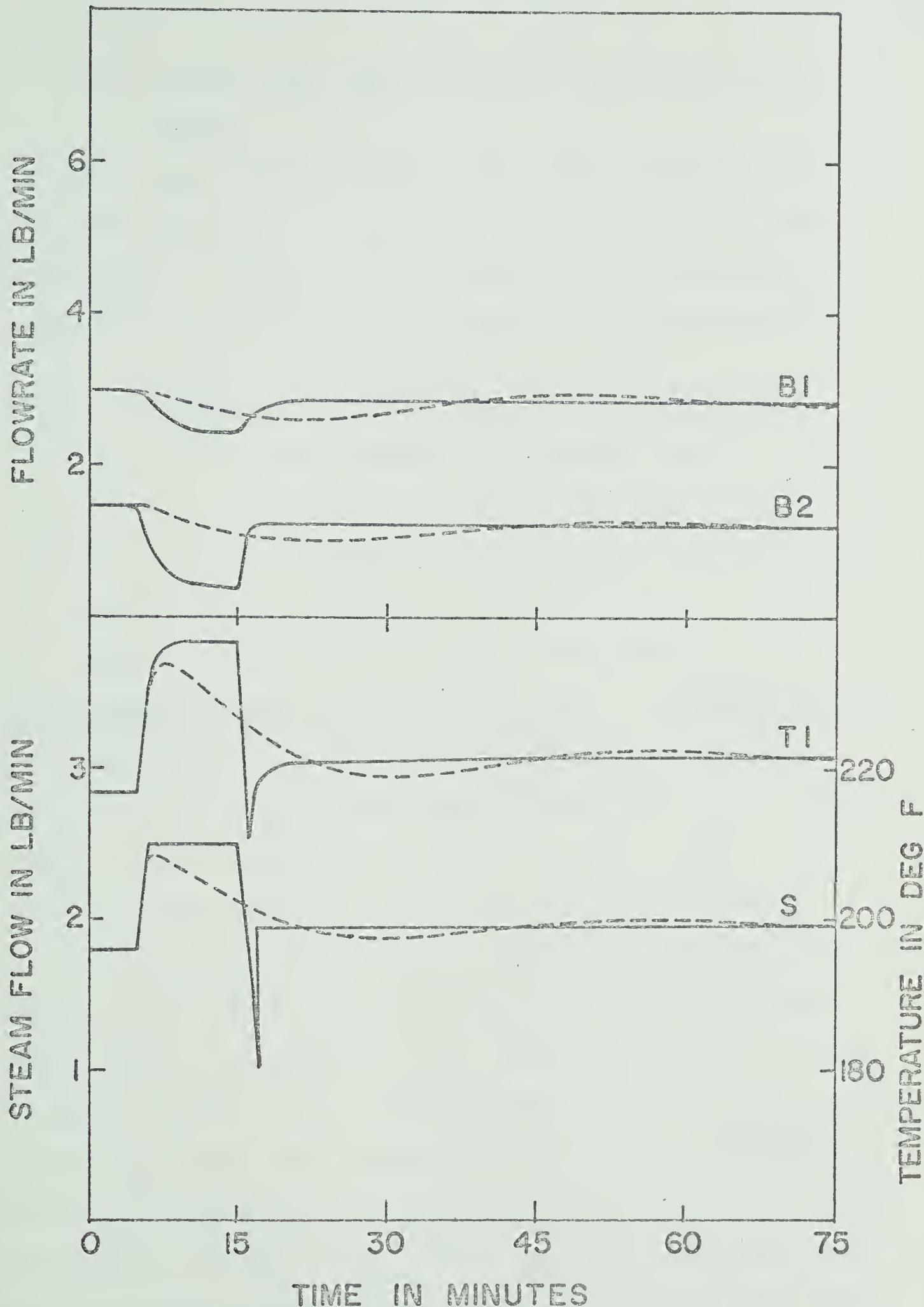


FIGURE 2b: Simulated Responses of Flow Rates and Temperature Under Optimal, Closed-Loop and Open-Loop Control
 — optimal, --- closed-loop, $\Delta\Delta\Delta$ open-loop

- (c) optimal open-loop state driving (second order model).

The significantly faster rise time and the shorter transient obtained in the optimal control case were the motivation for further investigation into the effects of model accuracy, constraints and physical implementation.

Case I: Optimal Control Based on a First Order Model

For a first order process the optimal control policy as developed in this paper is simply to step the input variable (S) to its maximum value and hold it there until the controlled variable (C_2) reaches the desired value. The input variable is then changed immediately to the value required for the new steady state. It should be emphasized that the optimal control calculation produces the switching time but does not estimate the value of the input variable required for the new steady state. (It must be found "by experience" or by using the model.)

The solid curve in Figure 3 shows the simulated response of the fifth order non-linear model to an optimal control policy based on a first order model fitted to the response of the same nonlinear model. At the precalculated switching point, the concentration is at the desired value and reducing the steam to the new steady state value should maintain C_2 at this value. Note the small overshoot that occurs due to "higher order" components of the fifth order model used in this simulation.

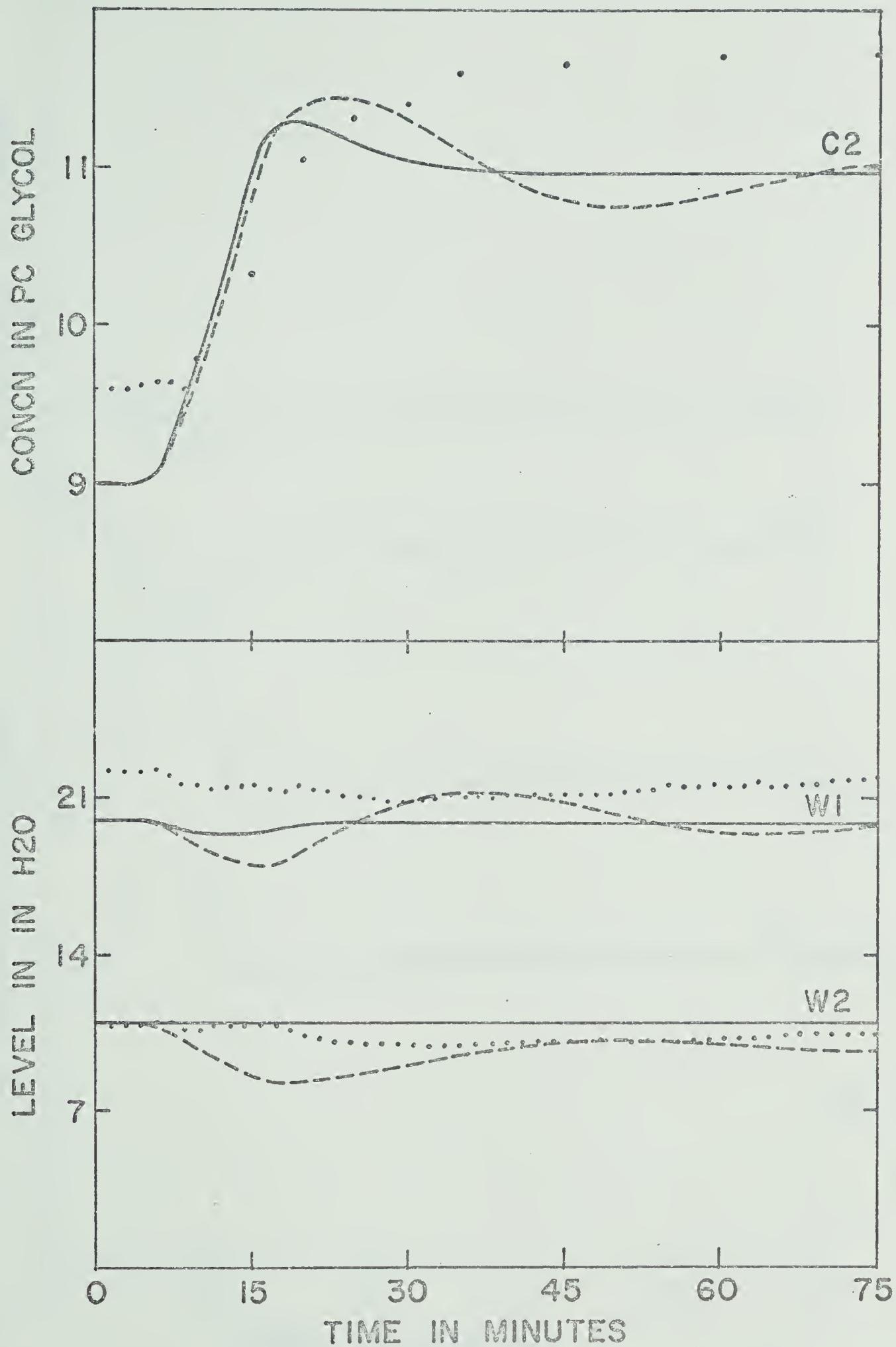


FIGURE 3a: Responses of Concentrations and Liquid Levels for Optimal Control Based on First Order Models
 — tight LLC, --- averaging LLC, ... experimental

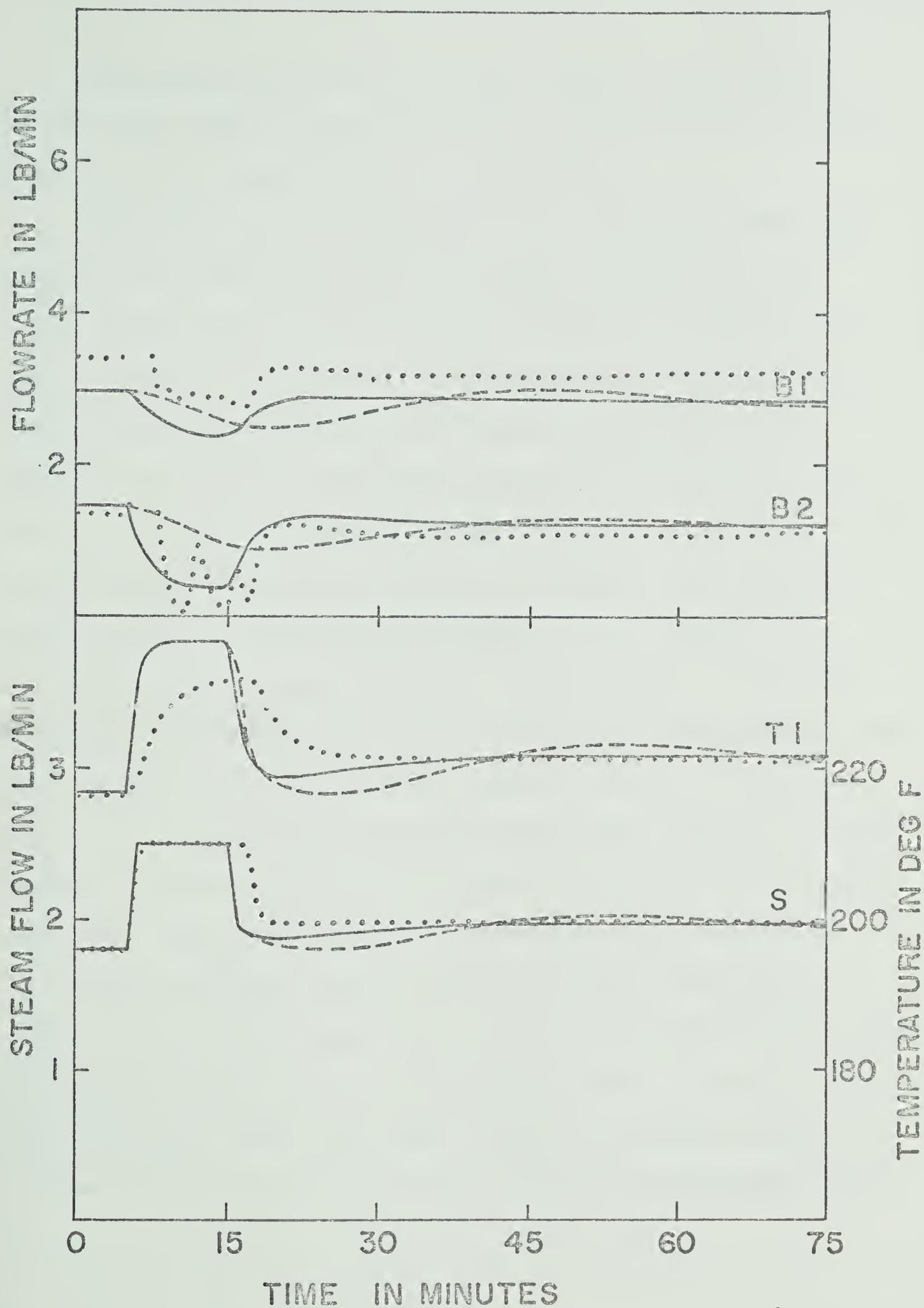


FIGURE 3b: Responses of Flow Rates and Temperature for Optimal Control Based on First Order Model
 — tight LLC, --- averaging LLC, ... experimental

The experimental and simulated results were plotted on the same graph to save space and not because the primary purpose was to compare the two responses.

The experimental response of the evaporator when subjected to an "optimal" steam transient based on a first order model fitted to the process response is shown by the points plotted in Figure 3. (Note that this experimental run was made with slightly different initial and final conditions.) At the time when the steam is switched to its final steady state value the concentration, C_2 , has only completed about 60% of its transient. However, the optimal control policy was based on a model of the form $K e^{-\tau_d s} / (\tau_1 s + 1)$ where $\tau_d = 5$ minutes, $\tau_1 = 39$ minutes, $K = 0.1085$ and $s_{max} = 2.5$ pounds per minute. Thus the value of C_2 that was reached due to the optimal control policy is found at $\tau_1 + \tau_d$, i.e. five minutes after the steam flow was reduced. However, even at this time the concentration has not reached its final value and continues in an open-loop response. It is obvious that a much better switching time could be found with a little experience. When the switching was done by actually measuring C_2 and switching when it was at the desired value, then there was a small overshoot, similar to the solid curve in Figure 3a, due to the "momentum (heat

capacity) of the actual process as shown by the solid curves in Figures 4 and 5.

The dashed and symbol curves in Figures 4 and 5 correspond to experimental response of the evaporator to DDC setpoint control and to a step change in steam to the new steady state value. Note that the setpoint change under the DDC regulatory control scheme results in violation of the pressure constraint in the first effect as can readily be seen by the temperature profile in Figure 5.

The true measure of the advantage of optimal control is obtained by comparing it with the conventional methods. "Conventional control" on the evaporator is implemented by using an inline refractometer to produce a continuous measurement of concentration which can be fed back to a standard P and I controller which manipulates the inlet steam flow. This scheme has performed satisfactorily for years as a regulatory control. However, in this investigation, where very large, rapid, changes were generated in flows and temperatures, it was found that the concentration readings were unsuitable due to temperature and flow interactions with the refractometer. Daily cleaning of the refractometer prism, careful calibration of the refractometer and accurate temperature compensation were required before on-line switching could be implemented.

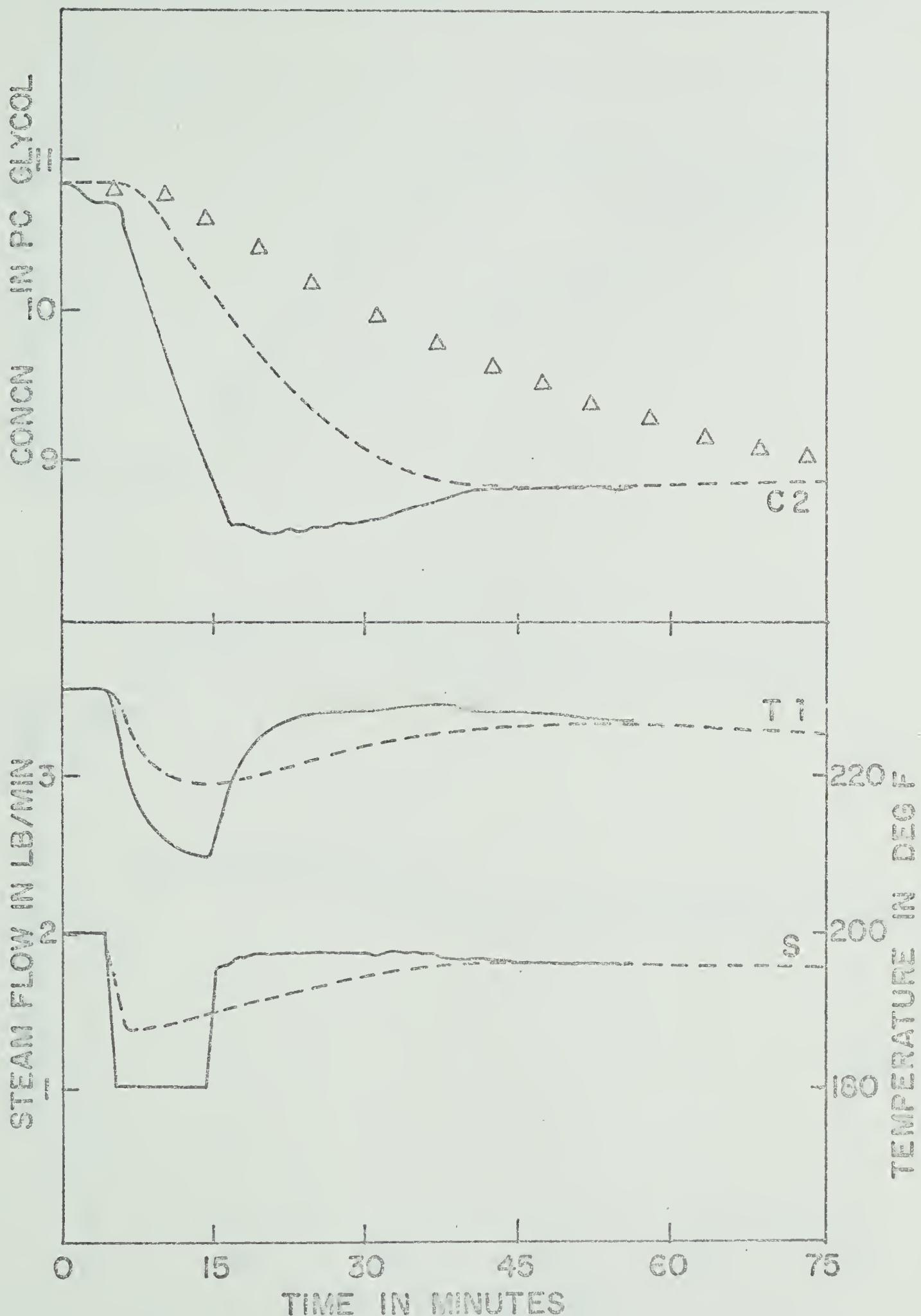


FIGURE 4: Experimental Response for Real-Time Switching Based on First Order Model
 — real-time, --- DDC feedback, $\Delta\Delta\Delta$ open-loop

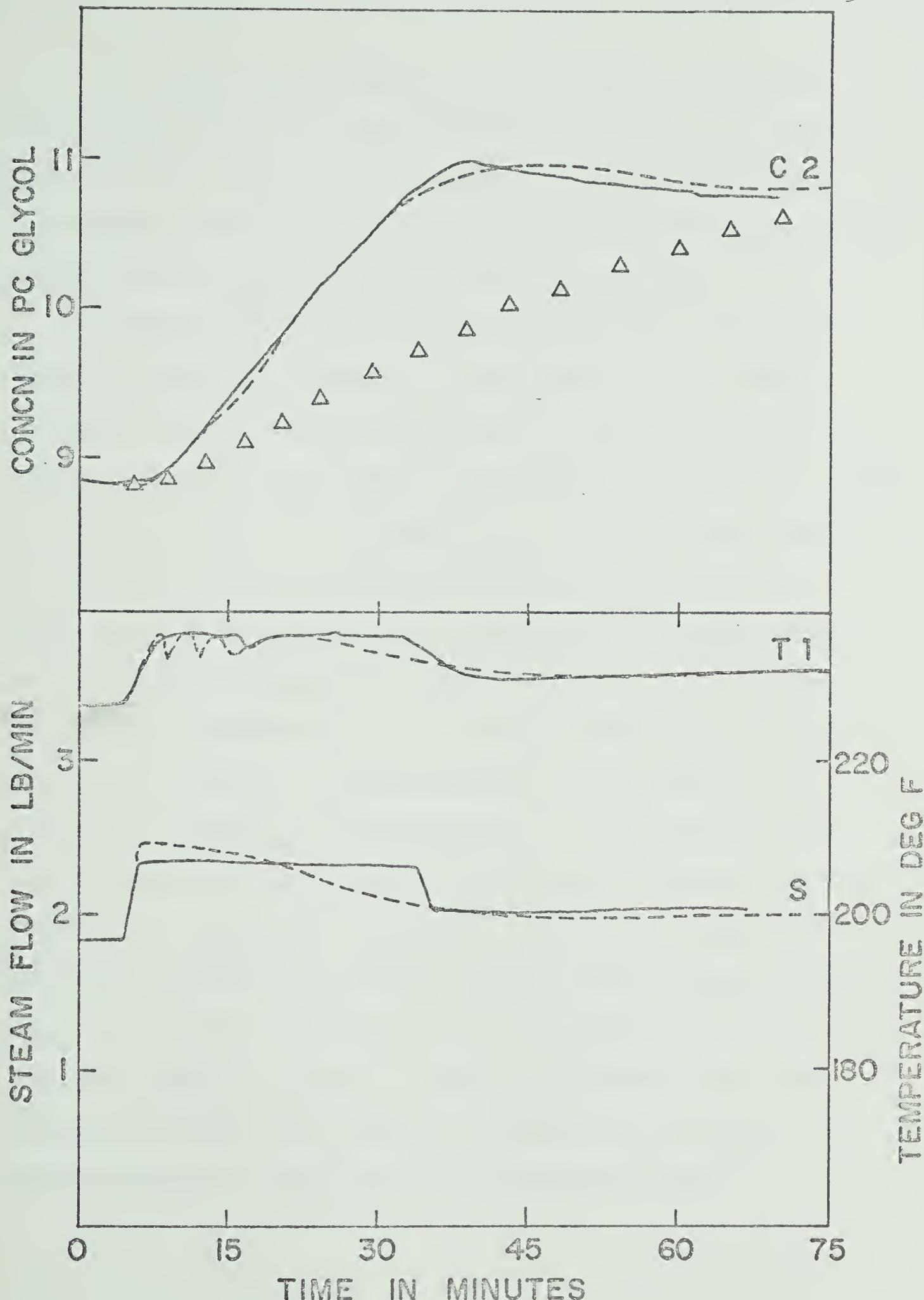


FIGURE 5: Experimental Response for Real-Time Switching
Based on First Order Model
— real-time, --- DDC feedback, $\Delta\Delta\Delta$ open-loop

This difficulty actually illustrates an important application area for open loop state driving, i.e. where the necessary measurement transducers are not available to produce readings fast enough or accurately enough, then open-loop procedures can be used to advantage.

Another refinement which developed from the experimental trials was a change in the liquid level control strategy. For standard regulatory control, it has proven advantageous to use P and I "averaging" rather than "tight" control on the levels ([16]p162) in the first and second effects, because this helps to damp out the effects of feed flow disturbances on C_2 . However, the large steam perturbations introduced by bang-bang control produced significant deviations in the liquid levels and these were very slow to be corrected as shown by the dashed line in Figure 3. Changing to relatively high gain proportional control on the levels for the duration of the state driving transient brought the evaporator to the new steady state (C_2 , W_1 , W_2 , etc.) in a much shorter time and was adopted for all the runs with the first and second order models. It does, however, produce larger variations in the manipulated variables B_1 and B_2 . An alternative solution to this problem is used in the multivariable cases.

Case II: Optimal Control Based on a Second Order Model

It was expected that the results obtained in Case I could be improved by using a model that would more accurately reproduce the process response and also make it possible to eliminate overshoot in the process (C_2) response. Accordingly, a second order model, equivalent to the transfer function defined by equation (3) was assumed. The parameters τ_1 and τ_2 were determined by using a computer program incorporating quasilinearization plus linear programming techniques to obtain the best fit between the state-space formulation of the model and the open loop response of the evaporator as discussed in Chapter Three. The results are shown in Table 1.

TABLE 1
PARAMETERS IN SECOND ORDER FITTED MODELS

Model	Fitted To	τ_1	τ_2	τ_d^*
1	Fifth order non-linear model	1.85 min	29.0 min	0 min.
2	Several actual process responses	12.1	20.2	0
3	Several actual process responses	7.8	22.3	3.0

* Specified by user

Models 2 and 3 have equally good criteria regarding "goodness to fit" but the theoretical model and other experimental data suggest that the smaller value of τ_1 in model 3 is more realistic. The simulated response of the fifth order model, when subjected to the switching times calculated from equations (5) and (6) and the parameters from the first model, is shown as the solid line in Figure 6. The manipulated variable (steam) is held at the upper constraint until C_2 almost reaches the desired value and then is reduced to the lower constraint value for a short time to prevent C_2 from overshooting. The overshoot is reduced from the simulated response in Figure 3. The steam was then set to the value equivalent to the new steady state (obtained from the model using non-linear gain). Note that the C_2 response differs slightly from the ideal, theoretical, response due to differences between the second order model and the "process" (i.e., fifth order model) and any error in picking the new steady state value for the steam.

The actual process response using switching times pre-calculated based on model 3 is shown by the points in Figure 6. The response of the outlet concentration, C_2 , is slower than that of the model (an observation supported by other data) but the change in C_2 from one steady state to another is smooth and fast. The process response using switching times based on model 2 are plotted in Figure 5 using dashed lines.

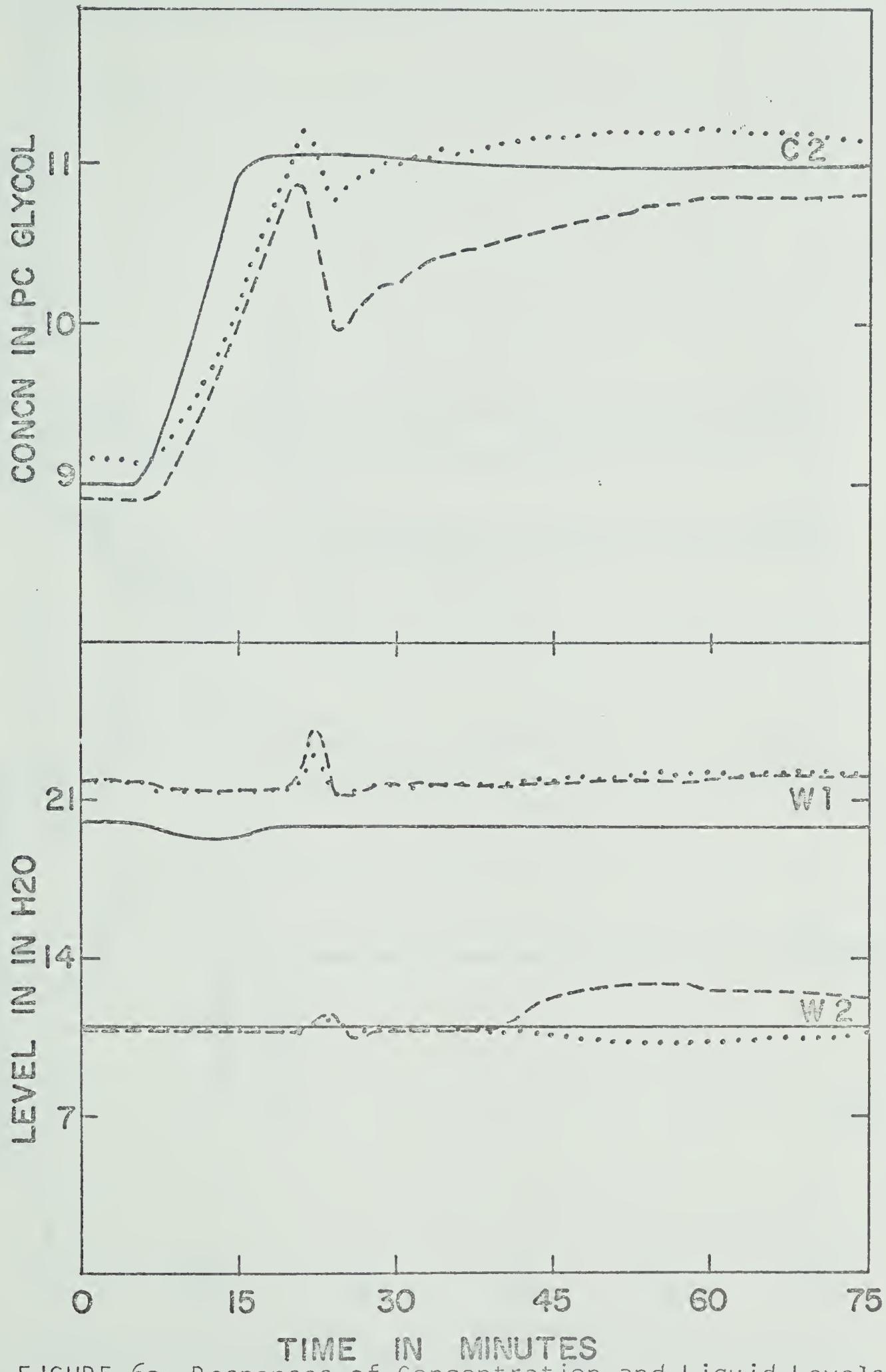


FIGURE 6a: Responses of Concentration and Liquid Levels
for Control Based on Second Order Models
— model 1(sim), --- model 2(exp. data)
... model 3 (exp. data)

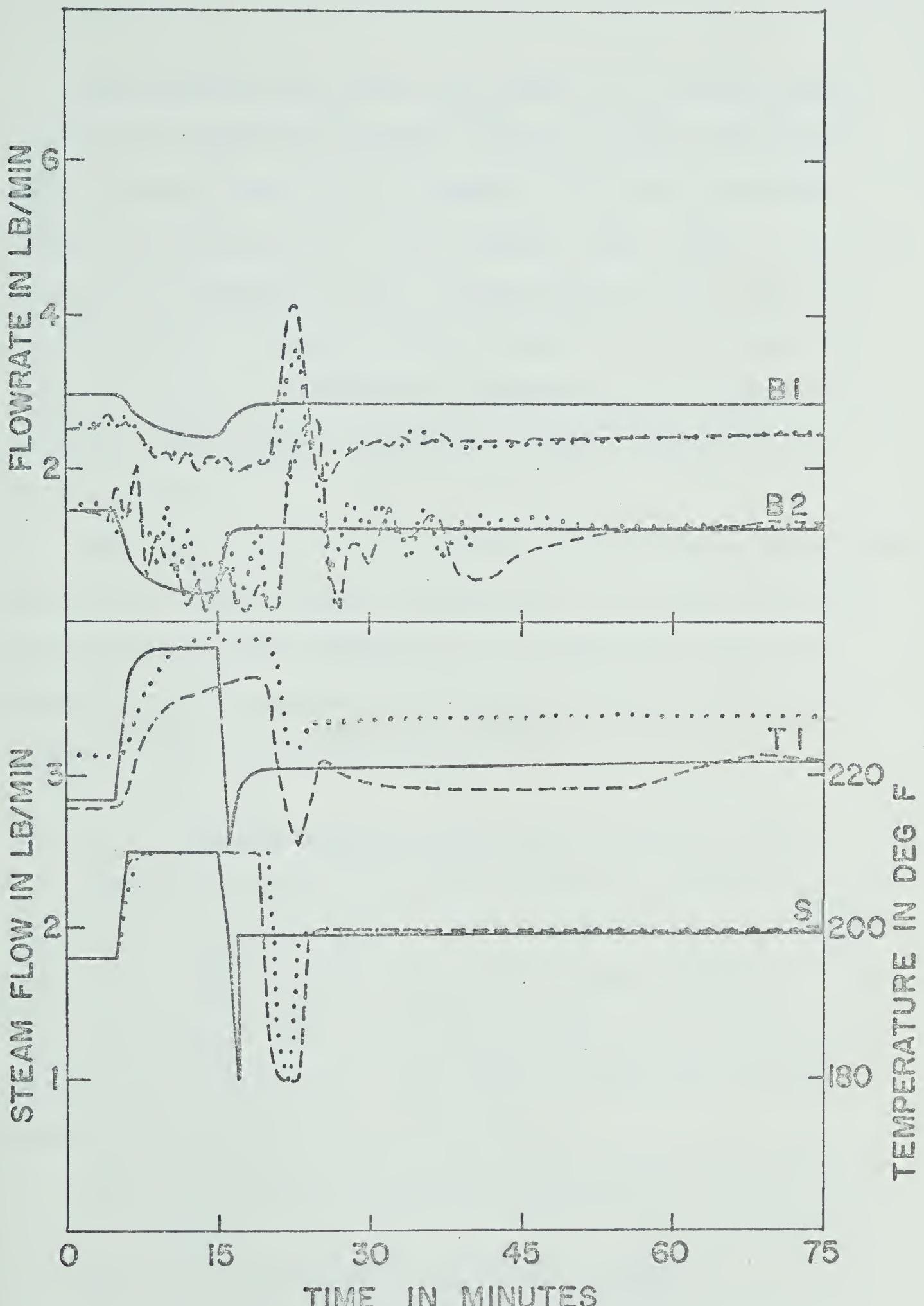


FIGURE 6b: Responses of Flow Rates and Temperature for Control Based on Second Order Models
 — model 1 (sim), --- model 2 (exp),
 ... model 3 (exp)

The decrease in C_2 and the peaks in W_1 and W_2 shown by both the dotted and dashed curves in Figure 6 are due to the steam remaining too long at the lower constraint before returning to the final steady state value. This in turn can be traced directly to the values of $\tau_1 = 12$ and $\tau_1 = 7.8$ found in models 2 and 3 respectively vs. the calculated value of $\tau_1 = 1.85$. This emphasizes the importance of "realistic" models rather than just a "good fit" to process data.

The liquid levels were under tightly tuned conventional control and stayed close to their setpoints. The large deviation in W_2 shown by the dashed curve in Figure 6 is due to a failure to achieve "bumpless" transfer back to the conventional P and I averaging control.

Case III: Optimal Control Using Real-Time Switching

Bang-bang control switching times calculated off-line are not always satisfactory due to modelling errors and/or real-time factors which affect the process response. Therefore two methods were investigated which would modify the switching times based on the actual response(s) of the controlled variables.

- (1) Analytical solution of the optimal switching curve.
- (2) An "intuitive" or empirical method.

In the analytical approach C_2 and dC_2/dt are estimated based on actual process measurements and the steam is switched when the actual trajectory in the phase plane crosses the switching curve. Athans and Falb [1] present a thorough treatment of the basis for this approach. It was not possible to implement this on the evaporator because the on-line estimates of C_2 and \dot{C}_2 were not reliable enough. The simulated results in Figure 7 show that the "real-time" implementation (solid line) moves directly to the desired value, whereas the results based on switching times calculated a priori from the same second order model (dashed line) show that the steam is switched too late (thereby causing overshoot in C_2) and then remains too long at the lower constraint (thereby causing over-correction in C_2).

Method one is ideal if an on-line computer is available to implement the switching and if satisfactory estimates of C_2 and \dot{C}_2 can be obtained. However, for manual implementation, the following method is more convenient:

- (1) calculate the optimal switching times from equations (5) and (6);
- (2) simulate the response of the system and determine the value of the controlled variable (C_2^*) at the first switching time and the length of time, Δt , the input variable is at the lower constraint (i.e., $t_2 - t_1$);

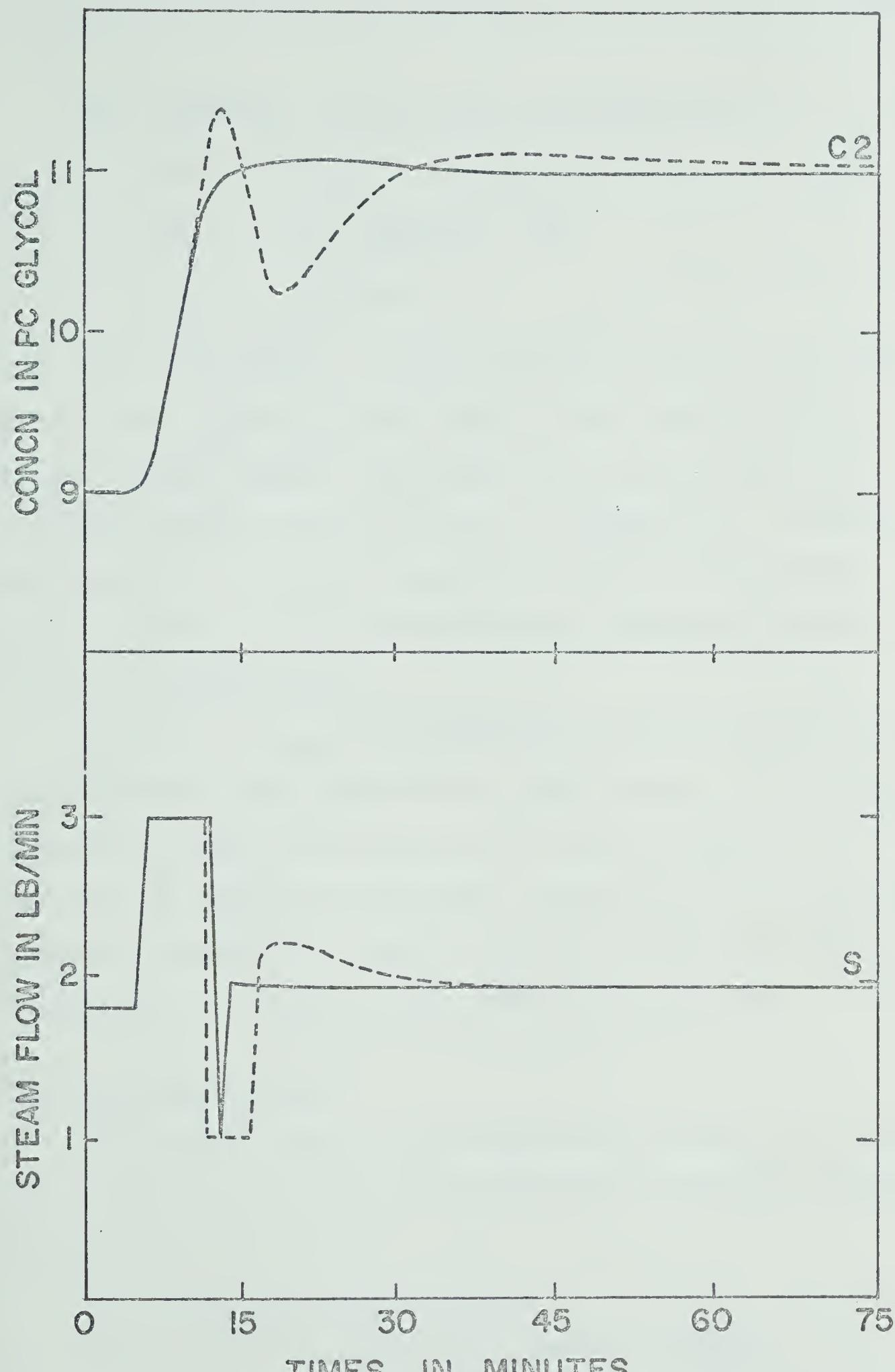


FIGURE 7: Simulated Responses for Real Time Switching
Based on Second Order Model
— real-time, ... precalculated

(3) implement the procedure experimentally

- (a) $S \rightarrow S_{\max}$ at $t = 0$
- (b) $S \rightarrow S_{\min}$ when $C_2 = C_2^*$
- (c) $S \rightarrow S_2$ after Δt .

The experimental results of Figure 8 and 9 show that "real-time" implementation (solid line) moves directly to the desired value. (Equivalent open and closed loop setpoint changes are also shown for comparison.) However the profiles in Figure 6 generated from pre-programmed control exhibit some overshoot and/or undershoot unless "tuned" to the process.

This is an empirical procedure and for a given process can undoubtedly be improved with experience. It must be emphasized that similar procedures can be implemented stepwise by making the allowable range $S_{\min} < S < S_{\max}$ small enough to guarantee a "safe" response and by switching a little early if there is any doubt about the time.

Multivariable Control

The single-input-single-output procedures used in Cases I, II and III are simple and convenient but do not properly account for:

- (1) multivariable processes
- (2) interactions between process variables
- (3) physical constraints on state or input variables.

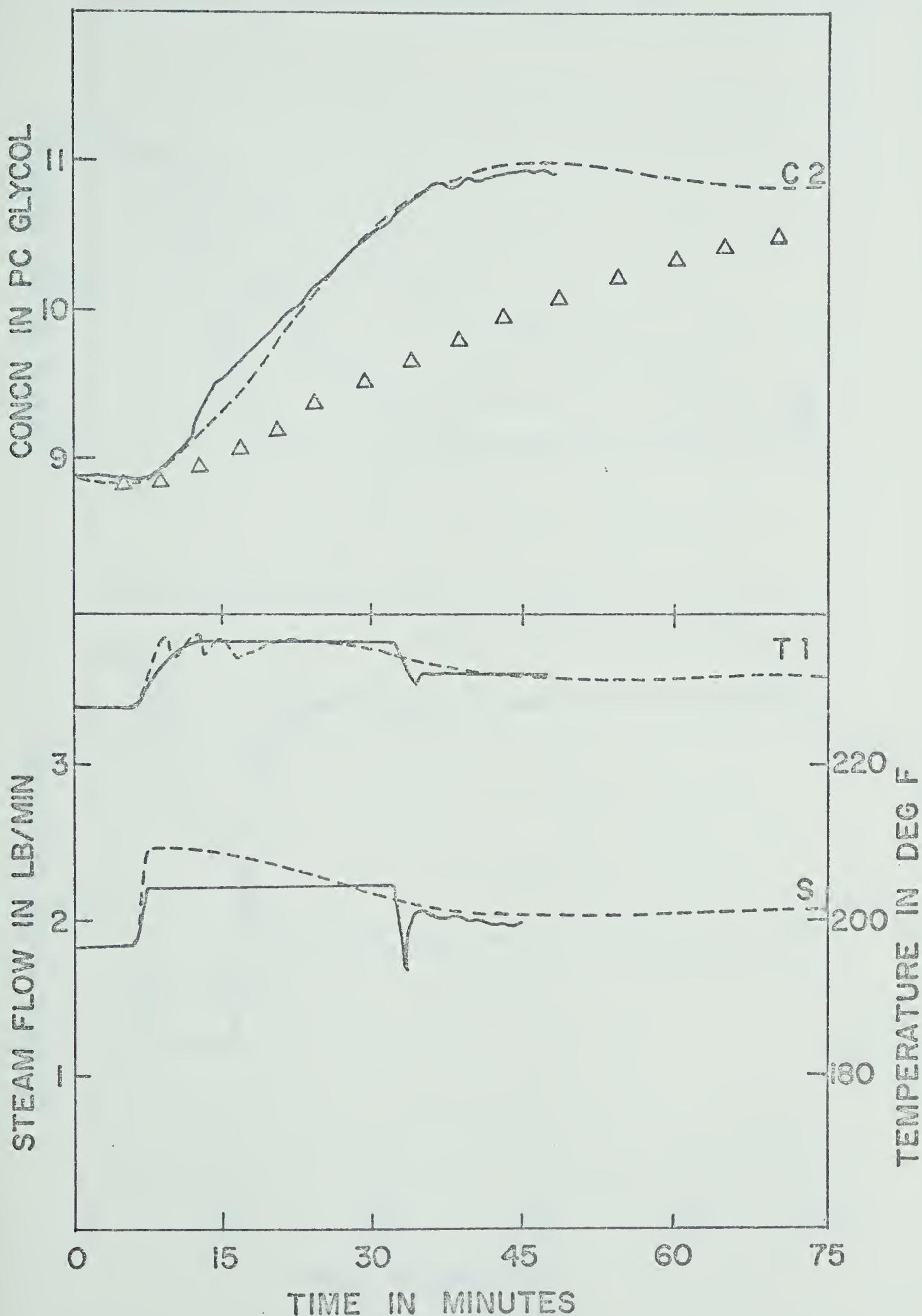


FIGURE 8: Experimental Response for Real-Time Switching Based on Second Order Model
 — real-time, --- DDC feedback, $\Delta\Delta\Delta$ open-loop

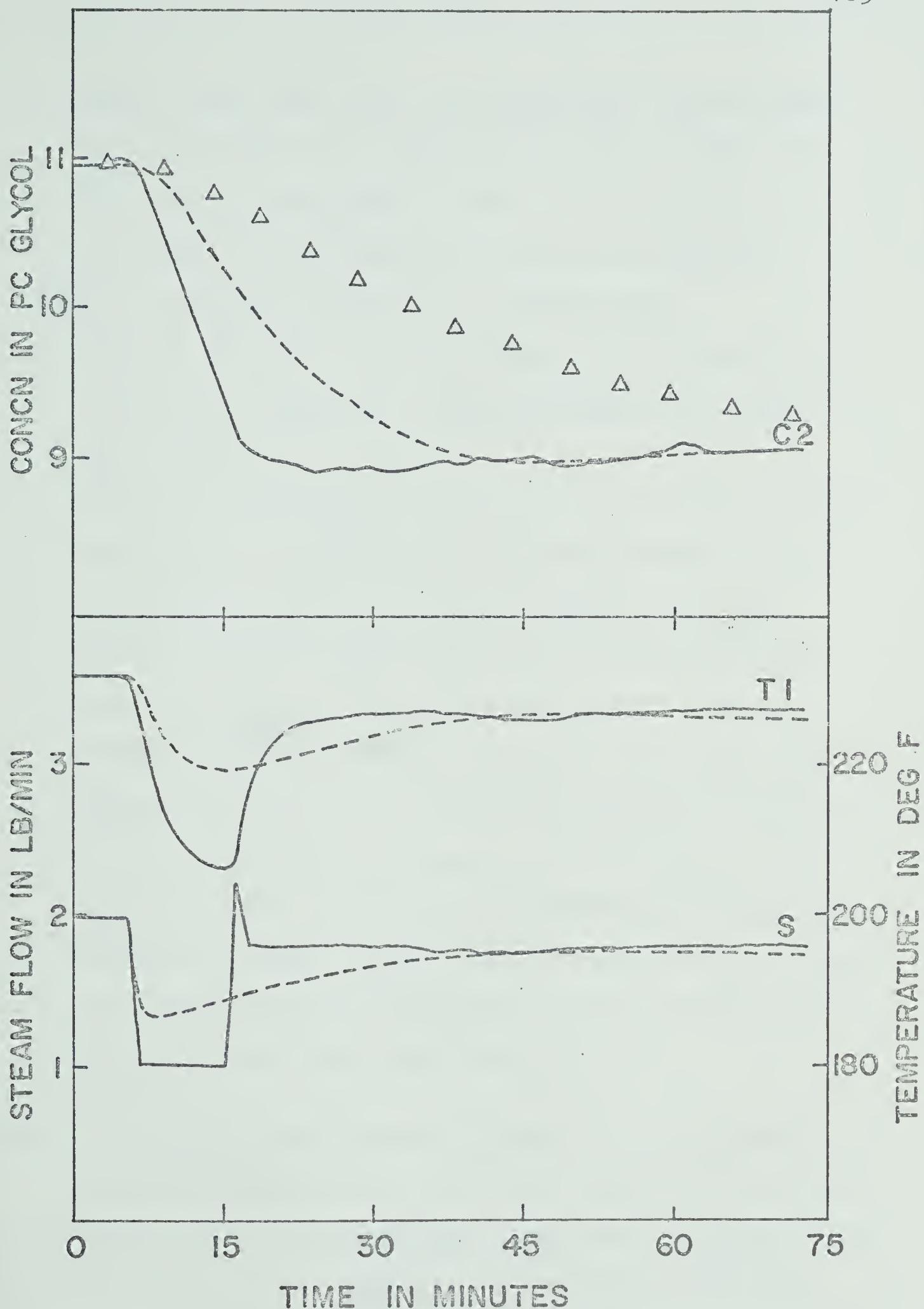


FIGURE 9: Experimental Response for Real-Time Switching Based on Second Order Model
 —real-time, --- DDC feedback, $\Delta\Delta\Delta$ open-loop

For example, experience with the evaporator showed that:

1. The stream from the first to the second effect (B_1) has almost as much and as fast an effect on C_2 as the steam, S , and therefore should be considered when calculating optimal C_2 trajectories.
2. Although they are not as critical, it is desired to drive W_1 and W_2 as well as C_2 to their new steady state values.
3. The high steam flows predicted by the simpler optimal control formulations cause the first effect to over-pressurize and blow the safety valve. (This was handled in the previous case by reducing the upper constraint S_{\max} on the steam flow and by running at a feed rate of 4.5 lb/min instead of the usual 5.0. However, it is a trial and error search to find the correct value and lowering S_{\max} extends the process response time). Therefore the investigation was extended to include optimal control based on the linearized fifth order process model and the linear programming formulation presented earlier.

Case IV: Multivariable Optimal Control of C_2 , W_1 and W_2

Results of optimal multivariable state driving based on a fifth order linearized model are shown in Figure 10. The dashed line is the response of the fifth order non-linear model, the solid line is from the response of the actual process. The optimal control policy is calculated

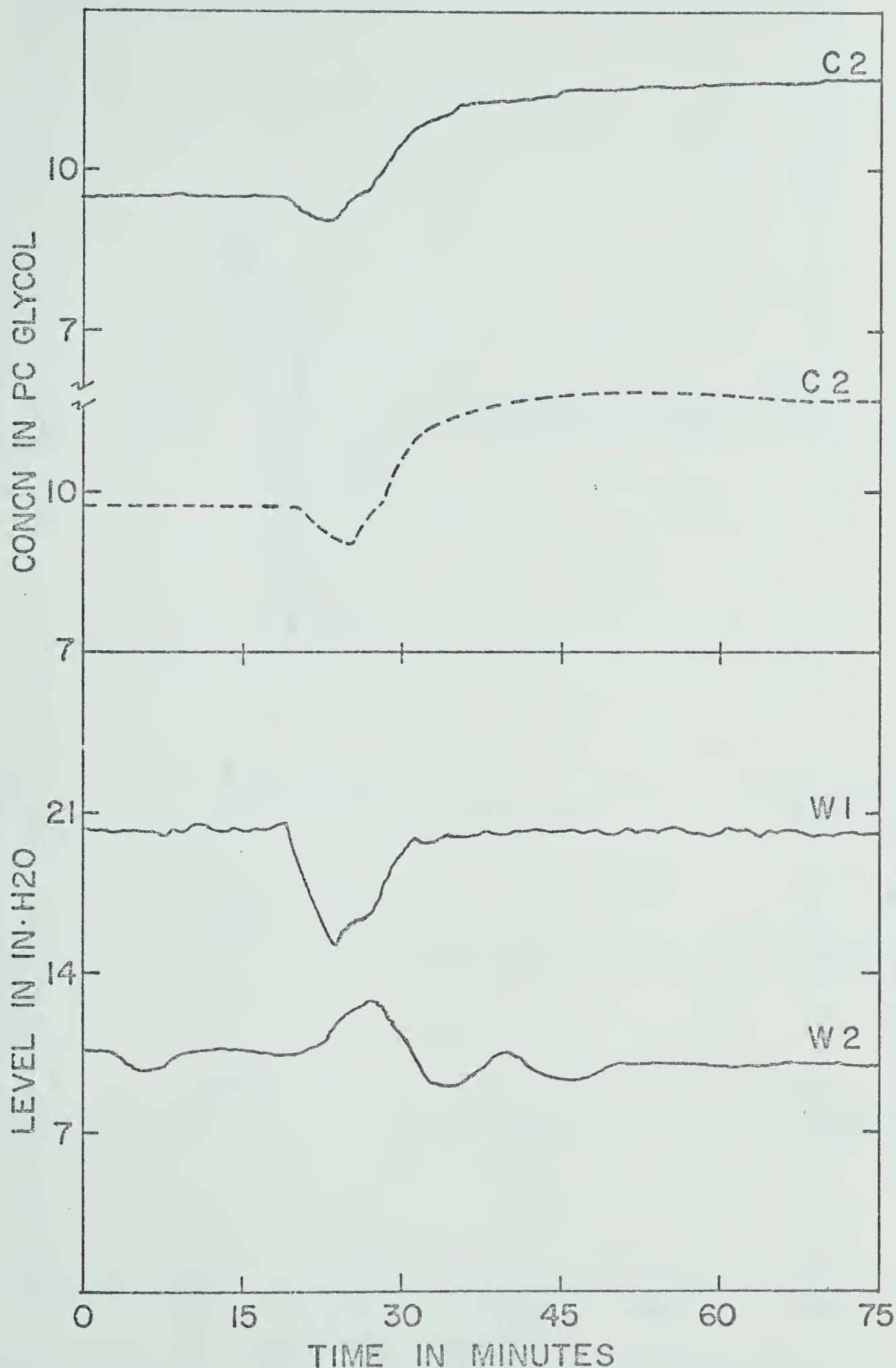


FIGURE 10a: Response of Concentration and Liquid Levels
for Control Based on Model 5L1 (IP - W₁, W₂, C₂)
— experimental, --- simulated

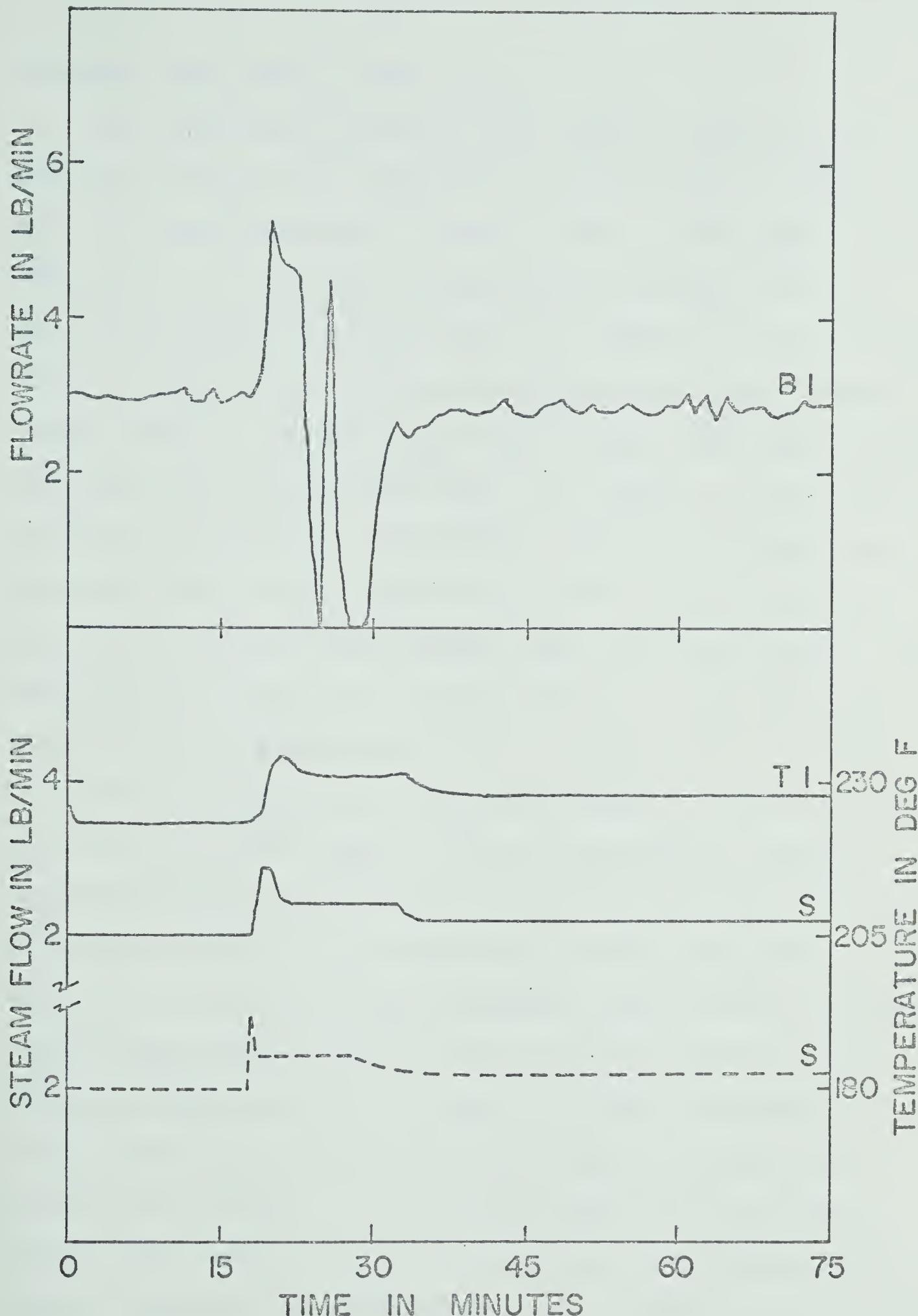


FIGURE 10b: Response of Flow Rates and Temperature for Control Based on Model 5L1 ($IP - W_1, W_2, C_2$)
 — experimental, --- simulated

from the fifth order linear model.

The controlled variables are steam, S , product from the first effect, B_1 , and product from the second effect, B_2 . The steam transient includes a step to the upper steam constraint at time zero, a step down to a lower value so that the process will not violate the upper limit on first effect pressure, (i.e., blow the safety valve) and finally a step down to the new steady state value. Note that within the resolution of the one minute time interval used in the numerical optimization calculations there is no step down below the final steady state value. The outlet flow B_1 and B_2 are also switched between their upper and lower constraints to return the liquid levels to their setpoint values (only B_1 is plotted).

The C_2 concentration trajectory shown in Figure 10 is distinctly different than in Cases I through III because of the bang-bang manipulation of B_1 and B_2 . Note particularly that the initial C_2 response is in the wrong direction. However - in spite of these "anomalies" the overall transient in the experimental runs is better (shorter) than for the single variable cases (ex. Figure 6). When comparing the actual experimental results for the single variable and multivariable cases it must be noted that the first and second order models were fitted to actual experimental responses, whereas the fifth order model is purely theoretical. It has been observed, in other work, that the response of

the fifth order model leads that of the actual process. Consequently the switching times calculated using this model are too "early" to fit the actual process response. A real-time switching scheme such as was simulated in Case III would definitely be of advantage here.

At the end of the state driving interval the variables were put back onto standard feedback control. However it was found desirable to put the liquid levels first onto high gain or "tight" liquid level control to quickly eliminate any residual error present after the state driving interval. The process was eventually returned to the averaging P and I control of liquid levels used for normal operations.

The same problem was also run without a constraint on the first effect pressure (actually an equivalent constraint on the first effect temperature). The simulated response (not presented here) showed the steam staying at the upper constraint instead of dropping down to an intermediate value and as a result the C_2 transient was significantly faster. This optimal control policy could not be implemented on the evaporator without exceeding the physical limit on the first effect pressure.

Case V: Multivariable Optimal Control of C₂

The objective in Case IV was to drive C₂ and the two liquid levels to the new steady state. This objective is overly severe since it is only necessary to keep the liquid levels within reasonable limits rather than return them exactly to their setpoints.

In Case V the liquid level performance was given zero weight in the objective function but upper and lower constraints were placed on the levels.

The experimental (solid) and simulated (dashed) results are shown in Figure 11. The steam trajectory is basically similar to Case IV but the manipulation of B₁ and B₂ is much less severe. Theoretically the response of C₂ should be better than in Case IV. However it is difficult to see any difference in the experimental results.

Once again the switching times were too "early" relative to the actual process response and could be improved significantly.

This ability of the linear programming formulation to handle zero weights on state variables is very important in practical applications because it makes it very easy to handle processes where some of the state variables are not directly observable and/or are not controlled variables. For example in the evaporator model the concentration out of the first effect is a state variable but there is no

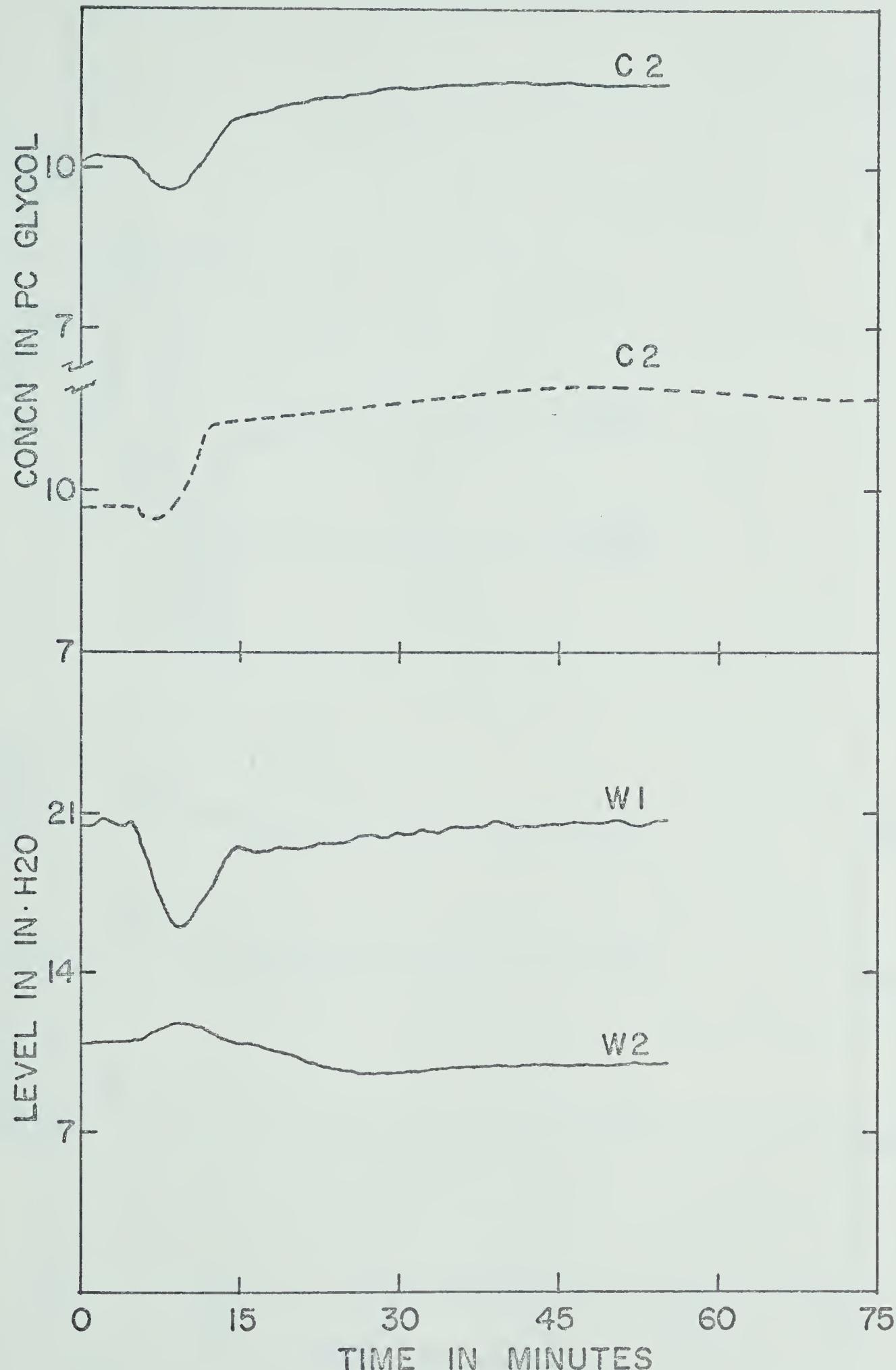


FIGURE 11a: Response of Concentration and Liquid Levels
for Control Based on Model 5L1 (IP - C₂)
— experimental, --- simulated

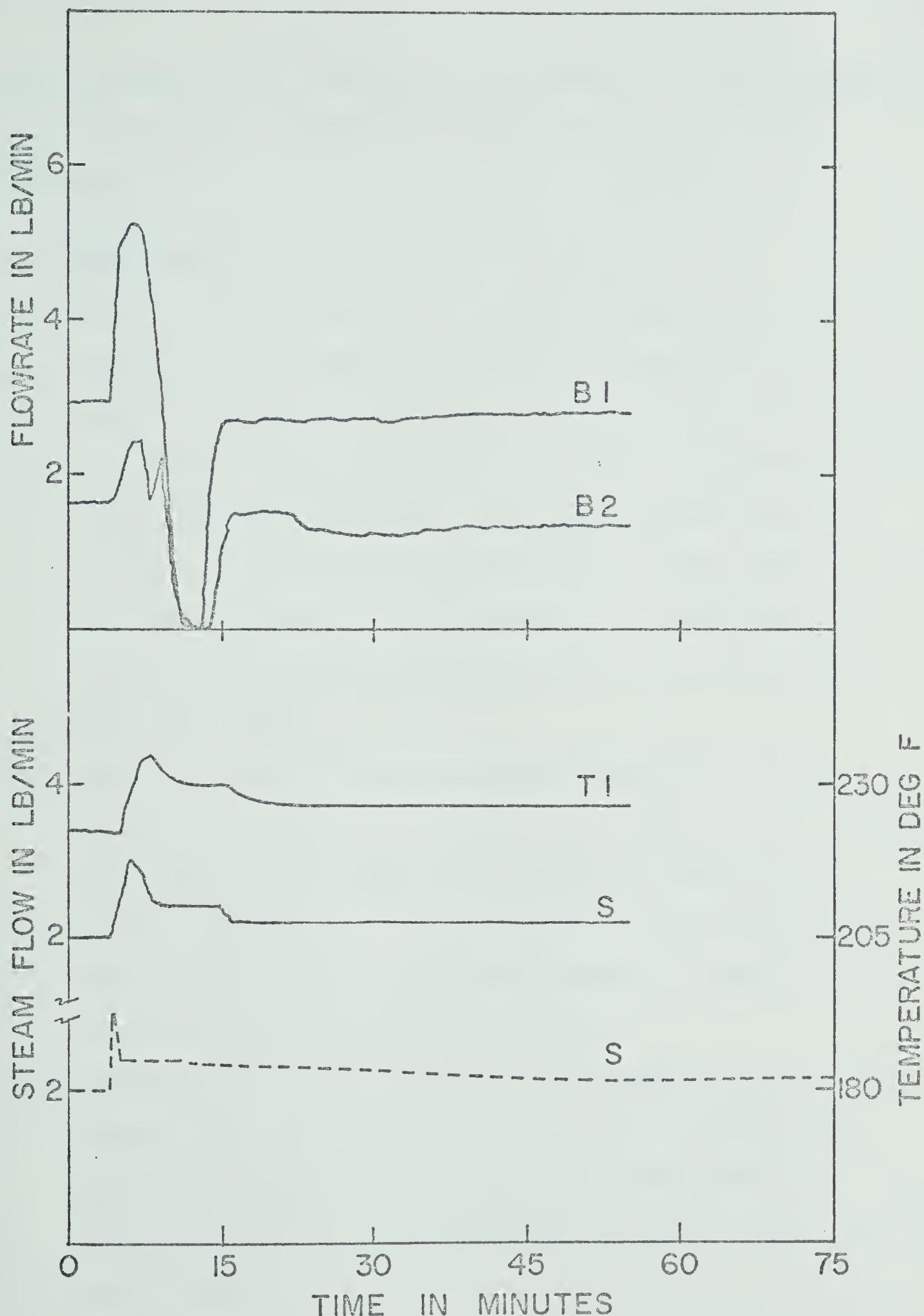


FIGURE 11b: Response of Flow Rates and Temperature for Control Based on Model 5L1 (IP - C₂)
— experimental, --- simulated

need to measure it, constrain it or specify a final steady state value for it when formulating the optimal control problem.

7. CONCLUSIONS

- (1) Optimal, open-loop state driving methods implemented manually or by computer control produced significantly improved responses for the pilot plant evaporator unit.
- (2) The linear programming formulation of the optimal control problem is flexible, practical and permits the direct introduction of constraints on the control and/or state variables. It is also applicable where all or only some of the state variables are of interest (or measurable).
- (3) Optimal control of the evaporator based on a first order fitted model was better than conventional methods but higher order models are capable of even better results and permit direct introduction of constraints. The "fitted" models in general produced better results than the purely theoretical models.
- (4) Combination of the optimal multivariable control techniques with conventional direct digital control of the pilot plant worked successfully and permitted improvements that were not practical when either was used alone.

- (5) If real-time measurements of the controlled variables are available then the switching times can be calculated or adjusted, to compensate for differences between the model and the process response.

CHAPTER FIVE

OPTIMAL STATE DRIVING CONTROL TECHNIQUES
COMBINED WITH CONVENTIONAL REGULATORY SYSTEMS:
AN EXPERIMENTAL EVALUATIONABSTRACT

Optimal, multivariable, state-driving control techniques were developed and implemented on a computer controlled evaporator pilot plant at the University of Alberta. The optimal control problem was formulated using a state difference equation model of the process and linear performance indices, including minimum time and sum-of-the-absolute errors, so that standard linear programming techniques could be utilized.

A method of adding the control policy developed from optimal state-driving techniques to a conventional feedback, regulatory control system was developed which simplifies the optimal control calculations, facilities implementation and, where possible uses the feedback action to compensate for modelling errors and disturbances.

Experimental and simulated results showed that the use of different criteria produced significantly different process transients and that constraints on the control and/or state variables can be incorporated to guarantee practical,

physically realizable control policies. The experimental results also showed that, although they are sensitive to model accuracy, optimal multivariable, state-driving control policies produce significantly faster setpoint changes than conventional methods. The method used to combine state-driving and regulatory control policies was practical and produced better results than either used alone.

1. INTRODUCTION

The purpose of this work was to develop, implement and evaluate optimal state-driving control techniques that would be suitable for use on industrial processes. A double-effect, pilot plant sized evaporator located in the Department of Chemical and Petroleum Engineering at the University of Alberta was selected for the experimental studies because of the large amount of information available from previous investigations and the fact that the unit was also interfaced to an IBM 1800 digital computer which could be used to facilitate data acquisition and implementation of more sophisticated control policies.

Several techniques exist to calculate optimal control policies [1]. The evaluation of these control policies by simulations using the control model results in dramatic improvements over conventional methods. However, when the objective is practical implementation on a real process then a number of additional factors, including the following, must be included:

(1) formulation of the problem

(a) Model: What complexity is required and how sensitive is the optimal process response to modelling errors? What process variables should be included in the model?

(b) Algorithm: The dynamic optimization algorithm should be able to handle a wide range of problems and to incorporate constraints on the state and control variables.

- (c) Criteria: Since a single criterion is unlikely to be suitable for all potential applications, the control engineer should have a choice of criteria and some indication of the influence of the criteria on the final process response.
- (2) combination of the optimal policy with existing regulatory controls

Since most optimal design procedures deal only with the control action needed to drive a process from its existing state to the desired state, the designer is frequently faced with the problem of how to combine the optimal state driving control policy with a separate regulatory control system. This problem is particularly relevant to existing processes, whether they are controlled by conventional or "optimal" regulatory systems. Modelling errors and unexpected disturbances must be anticipated and accommodated and the extra mathematical complexities involved with using closed, versus open, loop models must be recognized.

These points and others, as they apply to the implementation of optimal state driving control techniques on a pilot plant evaporator, are considered in the following sections.

2. LITERATURE REVIEW

In the optimal control literature emphasis has been placed on the quadratic and time optimal performance criteria because of the convenience of mathematical analysis.

For single loop servomechanism applications Latour et al [2] have presented analytical expressions for the time optimal switching times for overdamped systems represented by a second order transfer function with a time delay. They report that this method results in significantly better performance than that obtained using a well tuned PID controller and that the improvement increases with the magnitude of the setpoint change [2]. However more sophisticated methods are required for multivariable applications.

The two most popular approaches for determining the optimal control policies of multivariable systems have been dynamic programming and Pontryagin's Maximum Principle [3]. Numerical solution [1] using search techniques, quasilinearization or invariant imbedding is usually required. These methods produce excellent results but often encounter numerical or dimensionality problems in real applications and are not easily adapted to constrained systems. Tabak [4] reviews the application of mathematical programming techniques in optimal control theory. A linear programming formulation offers the advantage of being able to handle large multivariable systems with constraints on the control and/or state

variables and is the only approach presented in this work. Zadeh and Whalen [5] first showed that the time and fuel optimal control problems could be reduced to linear programming problems for linear discrete time-invariant systems. Bondarenko and Filimonov [6] present numerical results using these criteria. In the Chemical Engineering literature, Lesser and Lapidus [7] performed a numerical study using linear programming of the time optimal control of an absorber described by six first order linear ordinary differential equations.

Little work has been reported on the use of linear programming techniques with criteria other than time and fuel optimal performance indices. Lack and Enns [8] formulate a minimax criterion as a linear programming problem and compute the optimal control of a model of a nuclear reactor with twenty-one state variables. Propoi [9] presents a numerical example involving calculation of the optimal control policy of an overdamped system with minimization of the transient response area as a criterion. This is equivalent to minimization of the sum of the absolute value of the error at all the sampling instants since there is no overshoot. Lorchirachoonkul and Pierre [10] use a criterion whereby the absolute values of the errors are weighted in both time and space for multivariable distributed-parameter sampled-data systems.

Constraints on the control vector are particularly easy to incorporate into the linear programming formulation. However state variable constraints are much more cumbersome. Lesser and Lapidus indicate how state variable constraints may be introduced however only control constraints were used in their numerical analysis.

State and control variable constraints were used in Chapter Four which dealt with the dynamic optimization of the open-loop response of state space model of the pilot-plant evaporator at the University of Alberta using a time optimal criterion and standard linear programming techniques.

3. FORMULATION OF THE OPTIMAL CONTROL PROBLEM

An optimal control problem involves development of a suitable process model plus selection of an optimization algorithm and performance criterion. These will be discussed in the following subsections.

3.1 Model

Although linearization about nominal process values may be required, most multivariable processes may be adequately represented by the following linear, time-invariant, state space model:

$$\dot{\underline{x}}(t) = \underline{A} \underline{x}(t) + \underline{B} \underline{u}(t) \quad (1)$$

The optimal control problem may be stated as the determination of the trajectories of the control vector, $\underline{u}(t)$, needed to drive the system from its initial state, $\underline{x}(0)$, to the desired state, \underline{x}_d , while minimizing a particular objective function. It is assumed that the system as defined by equation (1) is state controllable.

3.2 Optimization Algorithm

Linear programming which is familiar to the process industries from other applications was selected as the optimization algorithm and the problem was formulated as follows.

Assuming that the control vector, $\underline{u}(t)$, is constant over the sampling interval, T , the analytical solution to equation (1) can be written in discrete form as:

$$\underline{x}(k+1) = \underline{\phi} \underline{x}(k) + \underline{\Delta} \underline{u}(k) \quad (2)$$

where $\underline{\phi}$ and $\underline{\Delta}$ are constant coefficient matrices determined by standard techniques [11].

Repeated use of equation (2) leads to the following sets of equations which permit the calculation of the state vector at each time interval in terms of the initial state vector and previous values of the control variables:

$$\begin{aligned}
 \underline{x}(1) &= \underline{\phi} \underline{x}(0) + \Delta \underline{u}(0) \\
 \underline{x}(2) &= \underline{\phi}^2 \underline{x}(0) + \underline{\phi} \Delta \underline{u}(0) + \Delta \underline{u}(1) \\
 &\vdots \quad \vdots \\
 &\vdots \quad \vdots \\
 &\vdots \quad \vdots \\
 \underline{x}(N) &= \underline{\phi}^N \underline{x}(0) + \underline{\phi}^{N-1} \Delta \underline{u}(0) + \dots + \Delta \underline{u}(N-1)
 \end{aligned} \tag{3}$$

This set of linear algebraic equations in conjunction with a linear performance index allows the use of standard linear programming techniques for solution of the optimal control problem.

3.3 Performance Criteria

Different criteria can result in significantly different responses and to date no one criterion or objective function has proven acceptable in all situations.

3.1.1 Single Point Criteria

Performance indices that have been used extensively in control system design, particularly for single output systems, include "time optimal", "minimax", and combinations of specifications such as percent overshoot and settle-out time.

The computational problem encountered in derivation of the time optimal control policy is to determine the minimum number of control intervals, N, within which the system can be driven to the desired steady state subject to any control or state variable constraints. This formulation and some of

the computational aspects were discussed in Chapter Four. The formulation is one in which only deviations of the state from the desired state at terminal time, $x_i(N) - x_{di}$, are of interest. The solution involves assuming a value for N and minimizing the maximum weighted deviation, λ , at time N.T.

This procedure is repeated using successively smaller values of N until λ can no longer be reduced below the limit specified by the user.

The minimax criterion requires that this minimum displacement of the state vector from an undesirable set of states, be maximized. This results in a linear programming problem similar to one iteration of the time optimal case except that all points in the state vector trajectory are considered in the objective function instead of just the terminal values.

A combination of specifications which is popular in process control is minimization of the rise time subject to limitations on the amount of overshoot and a specification on settle-out time. The minimum rise time can be accomplished in linear programming formulation by minimizing the (weighted) displacement of the state vector from its desired value at some selected point which falls in the interval between the start of the transient and the time at which any element of the state vector first equals the desired value. The limits on the overshoot (and subsequent "undershoots") are handled by state constraints applied for intermediate values of time, and the settle-out time is forced by tighter state constraints specified at later values of time.

Thus it can be seen that the linear programming approach permits one formulation to handle all three criteria. The only difference is in the weighting factors assigned to the deviations of the state variables from their desired values at different sampling instants.

3.3.2 Integral Criteria

Most modern design methods for optimal control of multivariable systems utilize a performance index of the following form:

$$J = \int_0^{t_f} F(\underline{x}, \underline{u}, t) dt \quad (4)$$

In conventional design methods the integral of the absolute error (IAE) index and the closely related integral of time multiplied by the absolute error (ITAE) index are popular linear integral criteria. The equivalent sampled-data criteria are the sum of the absolute errors (SAE) and sum of the absolute error times the time (STAE) indices. The criteria for the optimal control problem would then be to minimize, Z:

$$Z = \sum_{k=1}^N \sum_{i=1}^n w_i(k) |x_i(k) - x_{d,i}| \quad (5)$$

where $\omega_i(k)$ is the weighting factor assigned to the i^{th} state variable at the k^{th} sampling instant. For the STAE index $\omega_i(k)$ could simply be k . If only $\omega_i(N)$, $i = 1, 2, \dots, n$, is nonzero then this results in the time optimal control problem which can be solved by iteration using successively smaller values of N .

Equation (5) may be easily transformed into the following form which is more compatible with linear programming:

$$Z = \sum_{k=i} \sum_{i=1} \omega_i(k) (\epsilon_{1i}(k) + \epsilon_{2i}(k)) \quad (6)$$

where $\epsilon_{1i}(k) = x_{di}(k) - x_i(k)$ when the displacement is positive and $\epsilon_{2i}(k) = x_{di}(k) - x_i(k)$ when the displacement is negative. Using equation (3) the linear programming problem is to minimize the performance index, Z , as defined by equation (6) subject to the linear constraint equations of equation (9) where for all $k = 1, 2, \dots, N$:

$$\underline{u}_L \leq \underline{u}(k) \leq \underline{u}_U \quad (7)$$

$$\underline{\epsilon}_1(k), \underline{\epsilon}_2(k) \geq 0 \quad (8)$$

$$\underline{e} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ 0 & 0 & \dots & 1 \end{bmatrix}_{n \times n} \quad (8)$$

3.3.3 State Variable Weighting and Constraints

Control constraints are mandatory for most practical problems. Constraints in the form of equation (7) may be added directly to the linear program without increasing the size of the basis [12]. In order that the model response be tailored to the process engineer's specifications, provision must be made for state variable constraints and unequal state variable weighting. State constraints may be easily added to equation (8) by simply putting upper limits on $e_{1i}(k)$ and $e_{2i}(k)$. This does not result in a significant increase in execution time as stated above with reference to the control constraints.

Addition of state constraints to the time optimal criteria, by contrast, results in increased execution time due to the number of rows in the linear programming problem as indicated in Chapter Four.

Constraints on the derivatives of the state may also be added through a finite difference approximation. This is useful for removing inter-sampling ripple [10] and implementing constraints on maximum allowable rates of change so as to "ease" into optimal control.

$$\boxed{\begin{array}{cccccc} & & & & & \\ & \overline{x} & \overline{\phi} & N & \overline{x} & o \\ & - & - & - & - & - \\ \cdots & & & & & \\ & \overline{x} & \overline{\phi} & S & \overline{x} & o \\ & - & - & - & - & - \\ P & x & | & P & x & | \\ & & & & & \end{array}}$$

11

$$\left[\begin{array}{cccccc} \frac{e_{2N}}{N!} & \frac{e_{22}}{2!} & \frac{e_{12}}{1!} & \frac{e_2}{2!} & \dots & \frac{e_N}{N-1} & \frac{e_1}{1!} \end{array} \right]$$

Equation (9)

3.3.4 Computational Aspects

When a linear programming problem contains more variables than rows, solution of the dual problem is more efficient. This concept can be utilized in the solution of the time optimal formulation if the number of state constraints is not large. It results in a significant saving in computer time. However examination of the dimensions of equation (9), which are $(N \cdot n) \times (n \cdot m + 2 N \cdot n)$, indicates the primal solution is more efficient since the number of rows is less than the number of columns.

4. COMPARISON OF CRITERIA - A NUMERICAL EXAMPLE

Lesser and Lapidus [7] used linear programming to determine the time optimal control for the six plate absorber shown in Figure 1. The inlet concentrations were used as control variables in order to maintain linearity but they were constrained so as to constrain concentrations to a feasible range.

Material balances around each plate combined with a linear equilibrium relationship result in a linear vector differential equation identical in form to equation (1) where [7]:

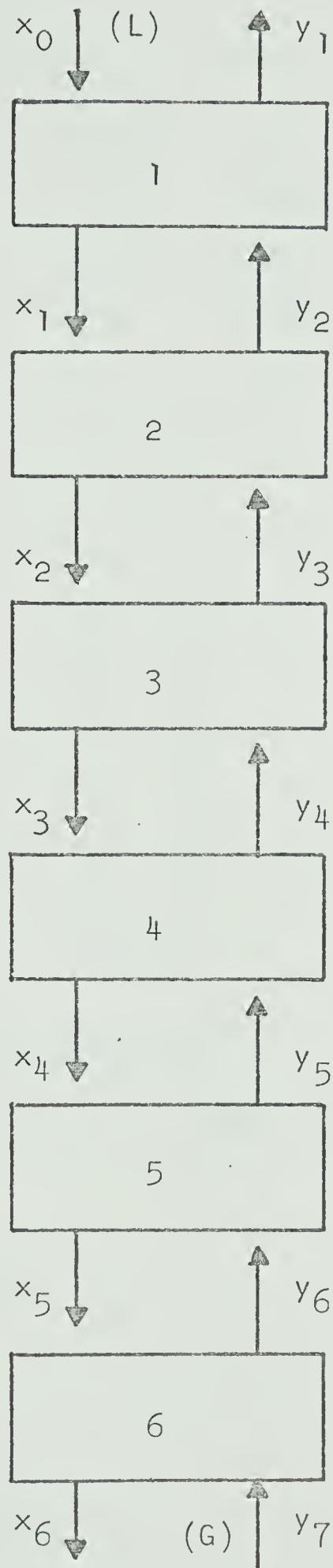


FIGURE 1: Schematic of Gas Absorber System

$$\underline{A} = \begin{bmatrix} -1.173 & 0.6341 & 0 & 0 & 0 & 0 \\ 0.539 & -1.173 & 0.6341 & 0 & 0 & 0 \\ 0 & 0.539 & -1.173 & 0.6341 & 0 & 0 \\ 0 & 0 & 0 & -1.173 & 0.6341 & 0 \\ 0 & 0 & 0 & 0.539 & -1.173 & 0.6341 \\ 0 & 0 & 0 & 0 & 0.539 & -1.173 \end{bmatrix} \quad (10)$$

$$\underline{B} = \begin{bmatrix} 0.539 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0.6341 \end{bmatrix} \quad (11)$$

The model is normalized such that:

$$\underline{x}^T(0) = [-0.0306 \quad -0.0568 \quad -0.0788 \quad -0.0977 \quad -0.1138 \quad -0.1273]$$

$$\underline{x}_i = \underline{0}$$

$$\underline{u}^T(0) = [0 \quad -0.1389]$$

$$\underline{u}(t_f) = \underline{0}$$

$$\underline{0} \leq u_1 \leq 1.0$$

$$-0.4167 \leq u_2 \leq 0.972$$

where the control variables are defined as:

$$u_1 = x_0$$

$$u_2 = \frac{y_7}{0.72} - 0.4167 \quad (12)$$

In Figure 2 the response x_6 (for a sample time of one-half minute) is compared for time optimal, SAE and the combination criteria. Note that, although the time optimal criterion is the only one which forced all the state variables to the new steady state in six minutes, the latter criteria yield "smoother" trajectories than does the time optimal criterion. These control policies are not unique [13]. The two SAE trajectories in Figures 2 and 3 result from formulations differing only in state variable weighting (equal weighting for all state variables (SAE1) versus the same weighting for all state variables except the product concentration which is weighted ten times the others (SAE2)).

It is of interest to examine the trajectories of the intermediate compositions as well. Figure 3 shows the trajectories for x_3 for the same three criteria. The intermediate trajectories in the combination criteria were not included in the objective function however the deviation from their desired steady state value was constrained. Note that the time optimal trajectory could be tailored to a more acceptable response through the use of state constraints on x_6 .

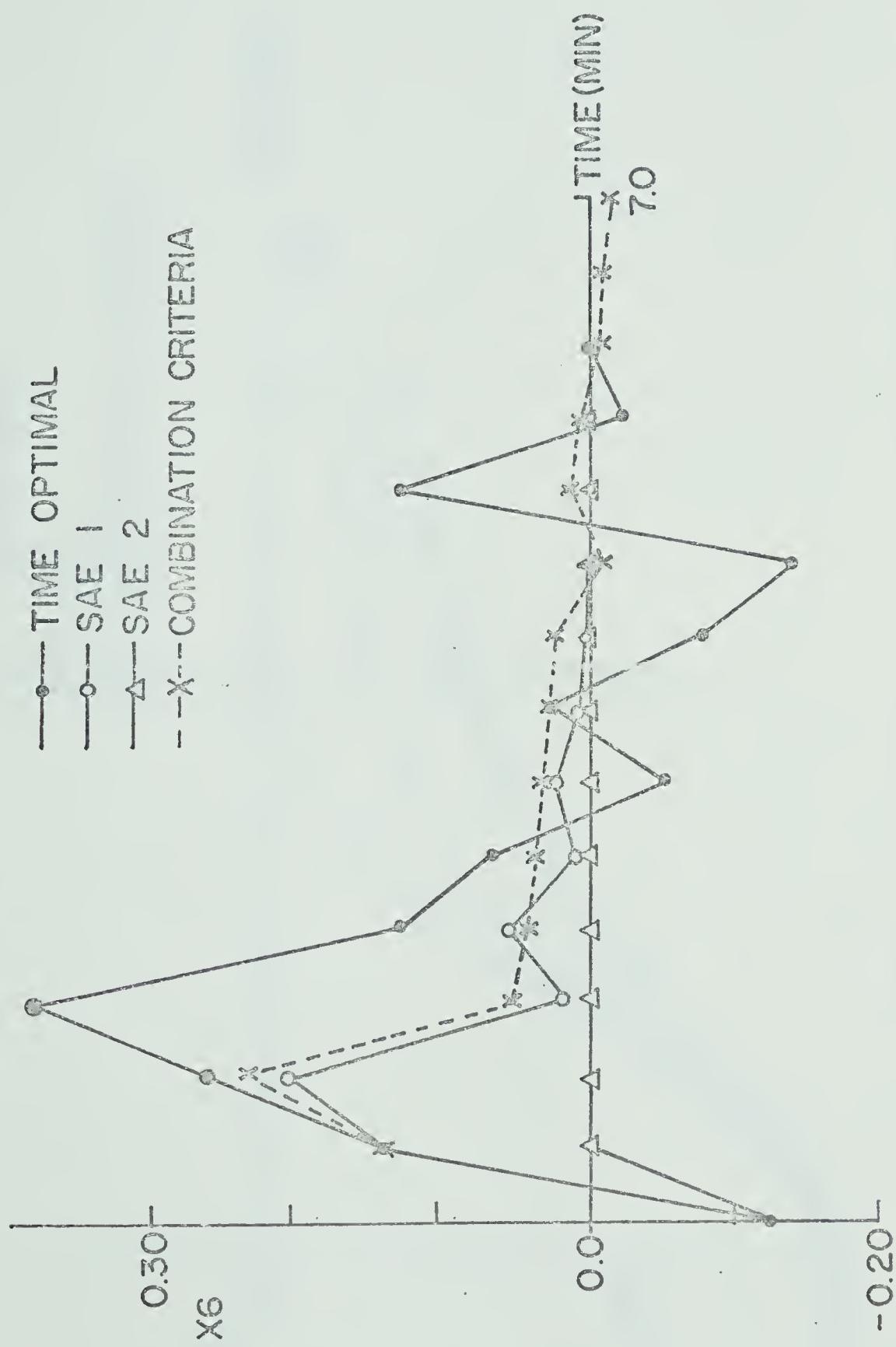


FIGURE 2: Response of x_6 for Different Criteria

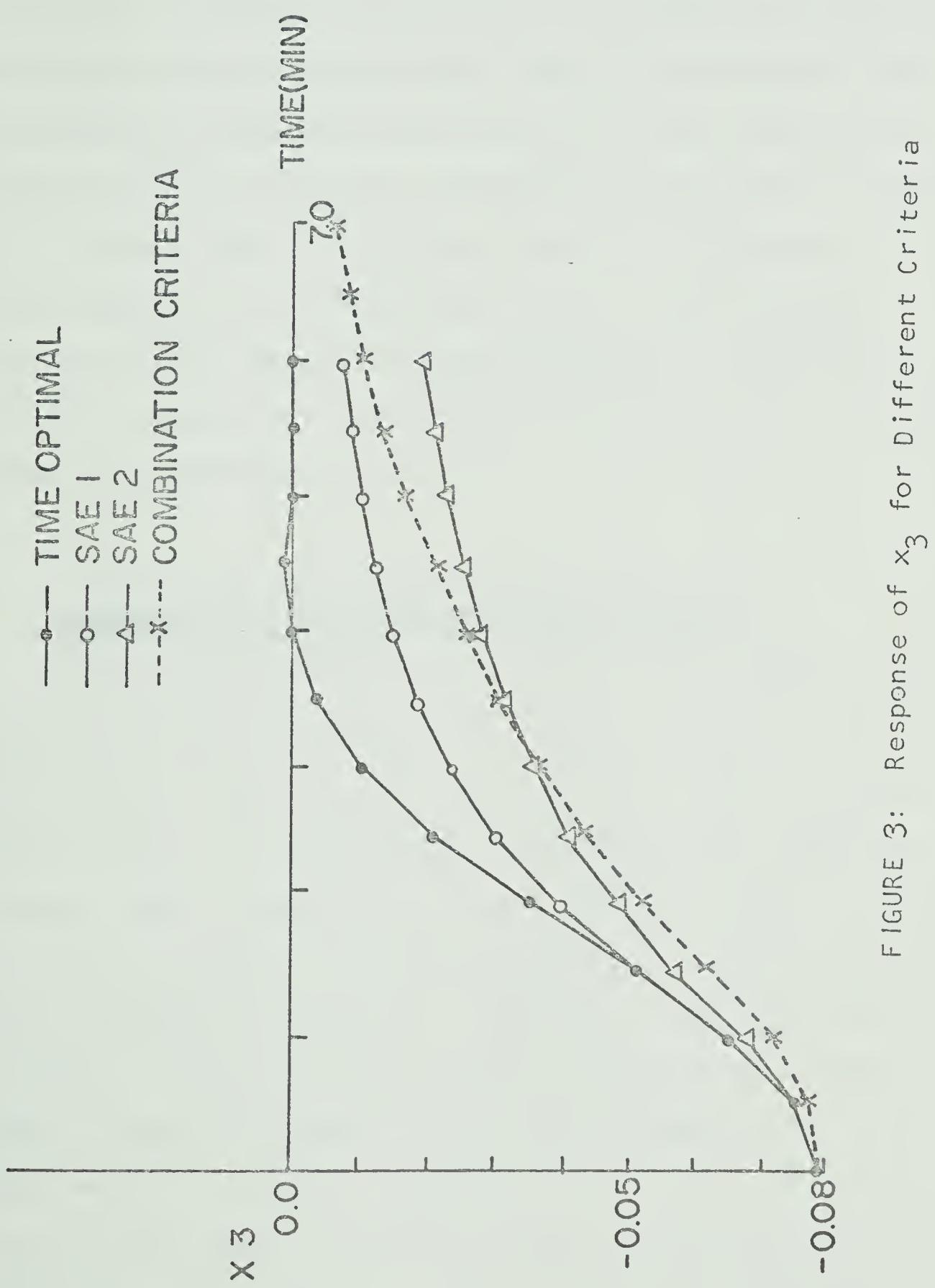


FIGURE 3: Response of x_3 for Different Criteria

This numerical example indicates the significant difference in response which may result from different criteria. The "best" choice of a performance index depends on the particular application. Through the use of linear programming techniques described in this work the process response may be tailored to desired specification by choice of criteria, addition of constraints and assignment of weighting factors to the state vector. Unfortunately design rules to generate weighting factors to produce a desired response are difficult to formulate and are usually chosen by experience.

5. INTERFACING AN OPTIMAL CONTROL SYSTEM TO A CONVENTIONAL CLOSED LOOP CONTROL SCHEME

Open loop implementation of the optimal control law can be used but modelling errors and disturbances may result in an offset from the desired condition. Some of these difficulties can be overcome by performing the setpoint changes under closed-loop control [14] by direct introduction of the step changes into the setpoints of loops "tuned" for the servomechanism problem. "Optimal" techniques require a model of the closed loop process which is more complicated than the open loop model because the elements of the control loop must be included. Locatelli and Rinaldi [15] discuss criteria for choosing between closed and open loop implementation of optimal control. Only in special cases can a rational *a priori* choice be made between the approaches.

The approach adopted in this work is to utilize the much simpler open loop model to derive the control law and to compensate for modelling errors or unsuspected load disturbances by interfacing the open loop control policy to the closed loop system in the manner represented schematically in Figure 4. When there is a priori knowledge of the nature, magnitude and time of the upset, load disturbances may be included in the model and compensated for by open-loop action. In the proposed approach the conventional feedback loop is not opened during the setpoint change but rather the predicted optimal state trajectories are feed to the setpoints of the corresponding control loops. Bumpless transfer can be effected at the beginning and end of each transient. If the process response, \underline{x} , and the optimal response, \underline{x}^* , are identical the feedback control action, \underline{u}_c , will be zero and the change in operating state will proceed in a fashion identical to the optimal open-loop implementation. In the presence of disturbances or model inaccuracies the control law is no longer optimal. However deviations from the calculated trajectory will be compensated for by the feedback control loops. Since the optimal state trajectory approaches the desired state at final time the system automatically returns to regulatory control.

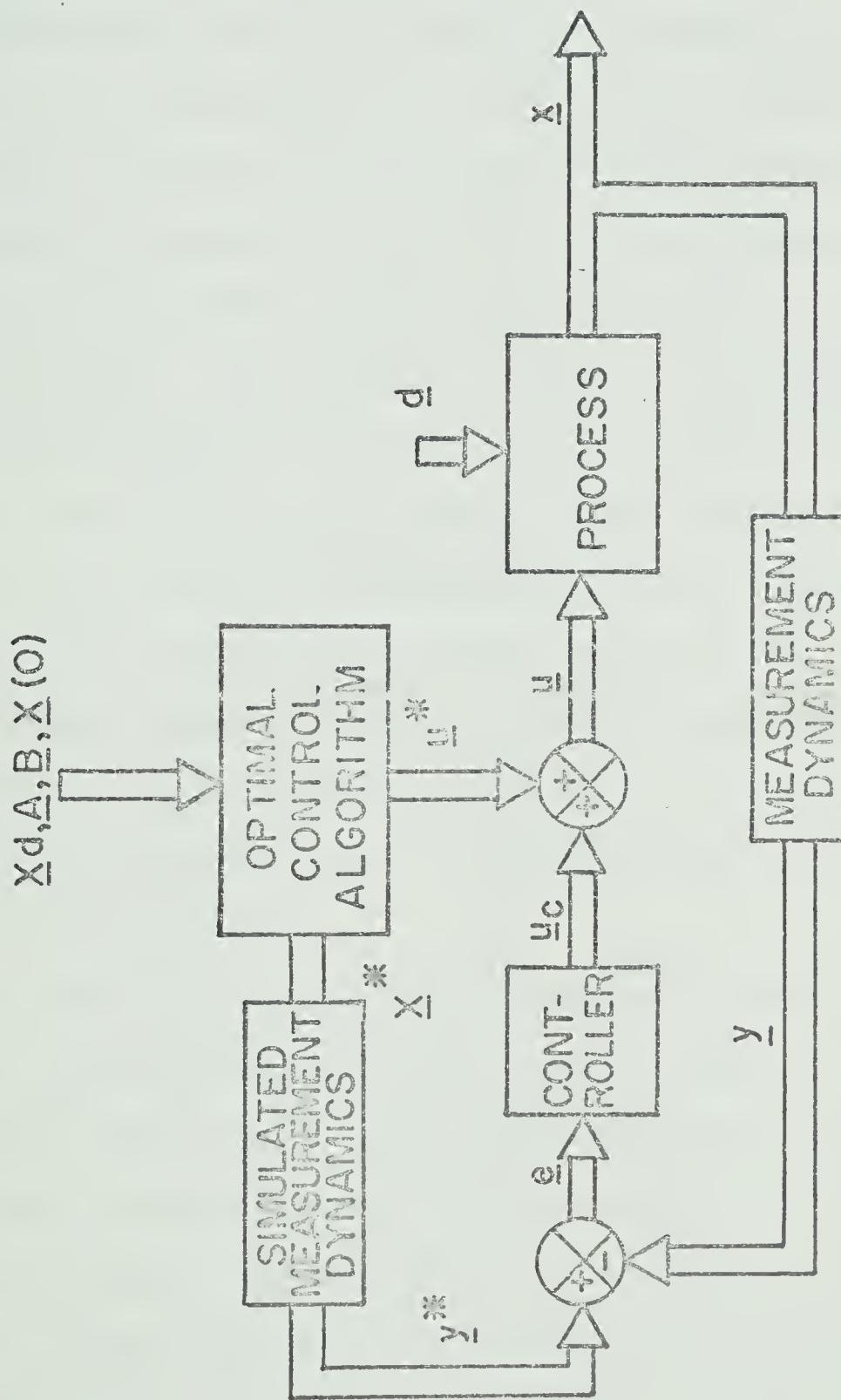


FIGURE 4: Addition of Open-Loop Optimal Control Policy to Existing Regulatory Control Scheme

6. IMPLEMENTATION ON A DOUBLE EFFECT EVAPORATOR SYSTEM

6.1 Process Description and Modelling

The optimal control techniques developed in previous sections were implemented on a pilot plant double effect evaporator equipped with conventional instrumentation. The measurement transducers and final control elements are interfaced to an IBM 1800 control computer which has a DDC monitor system. The process computer was used to facilitate data acquisition and reduction and implementation of optimal control. The process and computer configuration are discussed in more detail in Appendix A. As indicated in Figure 5, the three major control loops of the evaporator are cascade control loops. The bottom flow rates from each effect are manipulated to control the respective liquid levels and the steam rate is manipulated to control the product concentration.

For modelling purposes the evaporator can be considered as two, lumped parameter first order systems in series. Neglecting steam chest, vapor space and tube wall dynamics, mass, heat and component balances around each effect result in six nonlinear ordinary differential equations [16]. However, energy accumulation in the second effect can be neglected since the pressure, and hence temperature, is tightly controlled. The resulting set of five nonlinear differential equations is discussed in Appendix C (model 5NL).

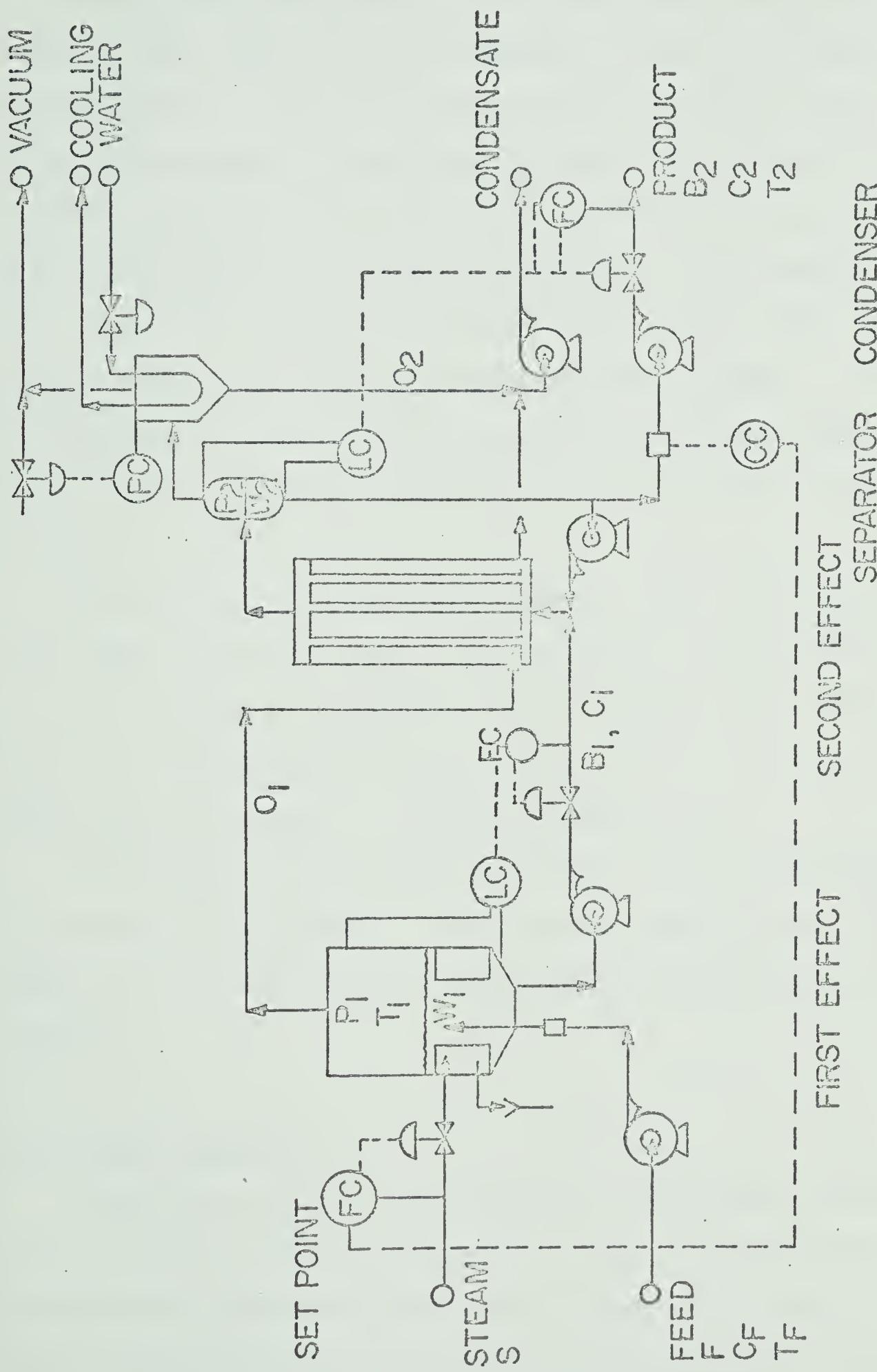


FIGURE 5: Schematic Diagrams of Double Effect Evaporator

Model 5NL exhibited a significant lead time when compared to the actual process response. Refer to Figure 2, Chapter Three. Since, as demonstrated in Chapter Four, an accurate model is necessary for open-loop state driving, the five equation nonlinear model was fitted to experimental data representing the process response to step changes in the steam rate. The fitted model (model 5NLF) exhibited considerably less lead than the theoretical model. Refer to Figure 2, Chapter Three. Details of the algorithm employed and problems encountered are related in Chapter Three.

The fifth order nonlinear models, models 5NL and 5NLF, were then linearized about nominal process values and put in the standard state space form of equation (1). The results are summarized in Appendix C. The linear models are referred to as models 5L and 5LF respectively.

The effect of improving the model accuracy by fitting the model to experimental data and the selection of the point to linearize about, are treated in subsections 6.3 and 6.4.

6.2 Model Reduction

Since the variable of interest is the product concentration, "optimal" single loop control may be implemented by manipulating steam flow while the liquid level loops are put under tight control as presented in Chapter Four. A second

order state equation, more commonly represented in the form of a transfer function of equation (13), can be used to approximate the relationship between steam rate changes and product concentration response:

$$\frac{C_2(s)}{S(s)} = \frac{K_p \exp(-\tau_d(s))}{(\tau_1 s + 1)(\tau_2 s + 1)} \quad (13)$$

However as demonstrated in Chapter Four, a "good" fit of this model to process data does not ensure good performance as a control model.

Table 1 summarizes some model parameters which will be utilized in subsequent sections.

TABLE 1
Various Model Parameters

	τ_d	τ_1	τ_2	K_p	USED IN FIGURE
Model 1	0	10	20	nonlinear gain*	11,12
Model 2	0	1.85	29	nonlinear gain**	13,14,17
Model 3	0	1.85	44	nonlinear gain*	6,15,16

* Appendix 1, Chapter Three

** $K = 0.0975$ used in Figure 13

The parameters for model 1 were chosen arbitrarily to give poor agreement; those for model 2 were fitted to the model response and those for model 3 to experimental data.

6.3 Evaluation of Theoretical and Fitted Models

In this section the performance of the theoretical and the fitted linear models will be evaluated using open-loop implementation so that feedback does not distort the effect of various models.

The control policies were implemented on the evaporator under program control synchronized with the DDC monitor. The three major control loops, as per Figure 5, are cascade control loops. During open-loop state driving the master loops were put on manual and the setpoints of the slave loops were provided by a control program [17]. A control transfer was then performed automatically at the end of the transient and the master loop reactivated [17].

The time optimal criterion was investigated first since it is practical and realistic. Since the product concentration is of prime concern, the other state variables were not included in the time optimal criteria. Rather the holdups were constrained to within 5.0 lbs of the steady state holdups and the first effect temperature was limited to the region less than 240°F. The first effect concentration is inherently constrained.

All setpoint changes are changes of two percent by weight in the product concentration (eg. from 9.0 to 11.0 percent glycol).

6.3.1 Control During State Driving ($0 < t < t_f$)

Figure 6 shows clearly how the response of the theoretical model, (5L), (dashed line) leads the process response (solid line). At the time the model response reaches the desired value the process has attained only sixty-five percent of the desired setpoint change. An intuitive way of looking at the discrepancy between the process and the model in Figure 6 is to regard the final switch line (arrow) to be approximately three minutes in error. With the rapid rate of change of product concentration this results in a large response error (approximately thirty-five percent).

From an intuitive point of view the optimal control policy for this problem of increasing the product concentration is to:

- (1) maximize the steam flow so as to maximize the boil off of water
- (2) minimize the bottoms flow from the first effect which reduces the dilution of C_2 by B_1
- (3) lower the second effect level to reduce the holdup and permit faster response.

These actions are evident in Figure 6 but are complicated by the state constraints. The steam flow increases to its maximum value and is almost immediately reduced to about 2.4 pounds per minute to avoid violating the constraint on T_1 . The levels perform as expected as can be seen from Figure 6.

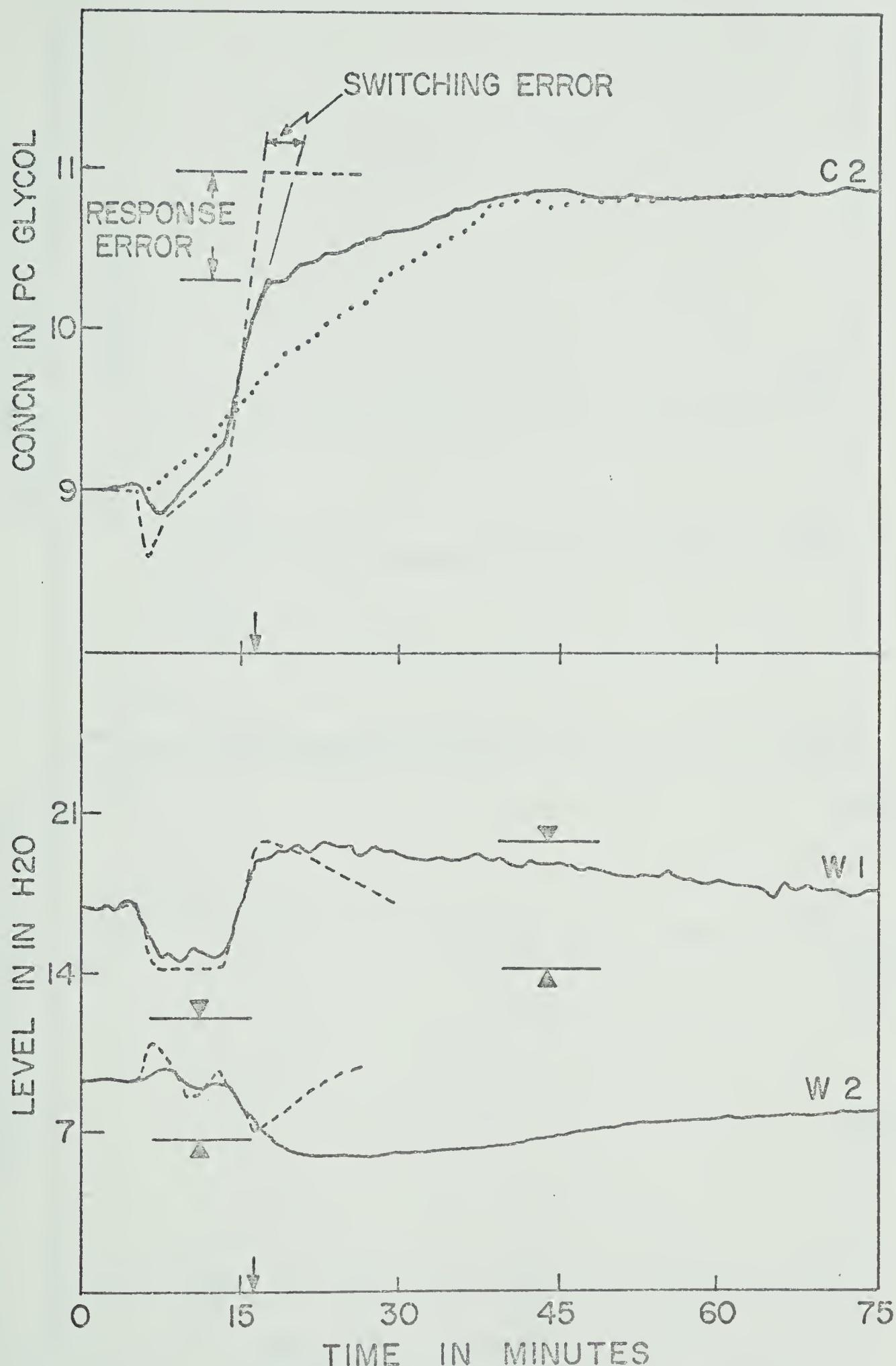


FIGURE 6a: Response of Concentration and Liquid Levels for Time Optimal Control
 --- model 5L, — experimental, Model 5L
 ... experimental empirical model



FIGURE 6b: Response of Flow Rates and Temperature for Time Optimal Control
 --- model 5L, — experimental, Model 5L

The constraints on the levels are represented by the horizontal solid lines with the solid arrows. The B_1 and B_2 control policies are not easily interpreted and are not unique.

The dotted curve in Figure 6a is the experimental process response produced from the time optimal control policy derived from model 3 of Table 1. The rate of increase of C_2 under the two different policies clearly shows the advantages of using the multivariable approach. Since all simulated (from 360 CSMP) and experimental data was recorded at one point per minute, and since these points were plotted on a calcomp plotter, some peaks are diminished and step changes take on a ramp like appearance. For example the initial spike in the steam response of Figure 6b is much reduced. Another contributing factor to this plot characteristic is the finite response time of the actual process variables.

The response displayed in Figure 7 is the result of the linearized model 5LF which was obtained from the nonlinear model, 5NLF, fitted to the open-loop response of the process to step changes in steam flow rate. Chapter Three details the results and procedure. Since the model more closely represents the process, better control is achieved. This can be seen from the reduced response error in the product concentration, approximately fifteen percent in Figure 7 compared to thirty-five in Figure 6. The dashed

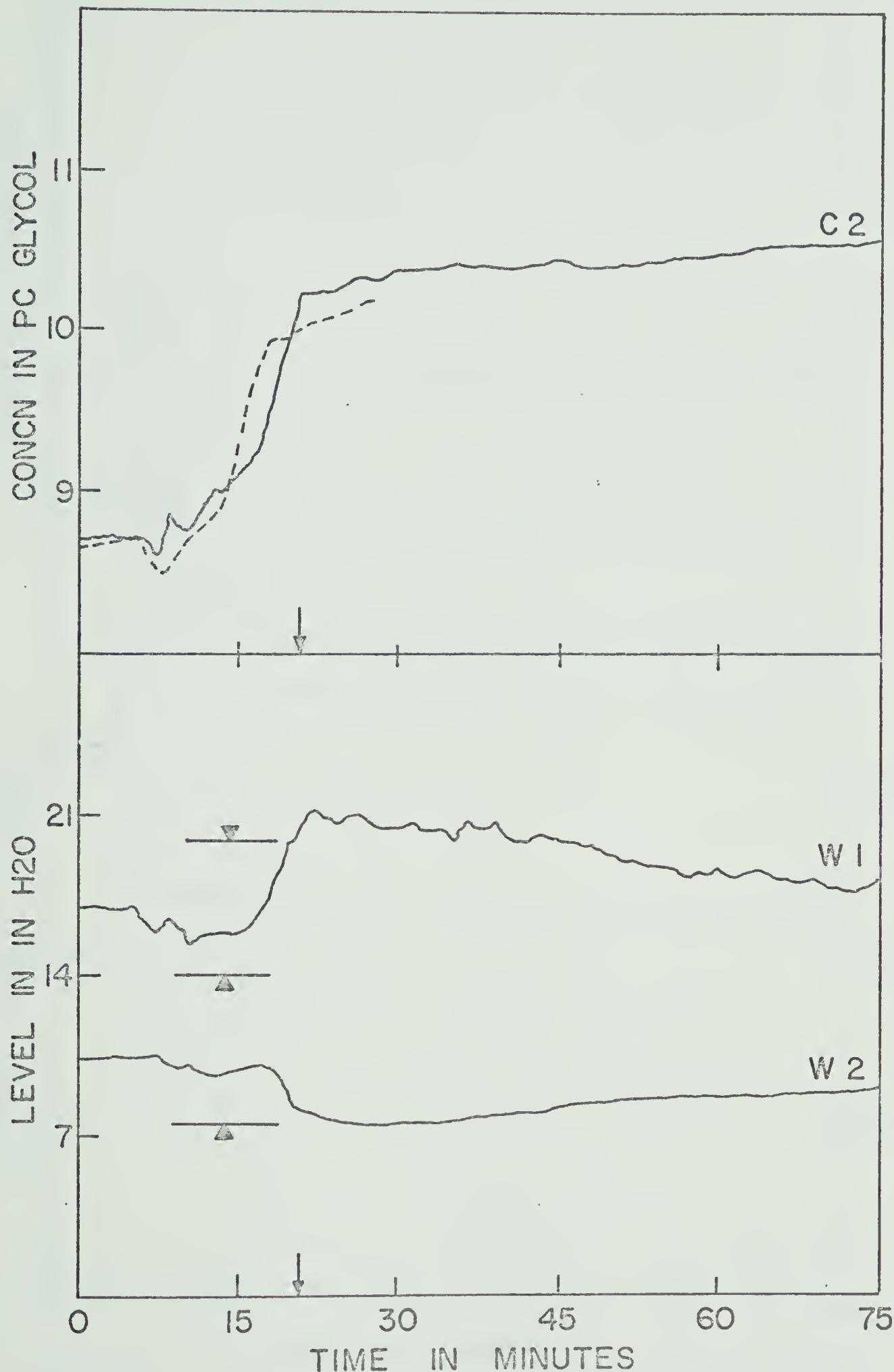


FIGURE 7a: Response of Concentration and Liquid Levels for Time Optimal Control
 ——experimental, Model 5LF, --- experimental Model 5L

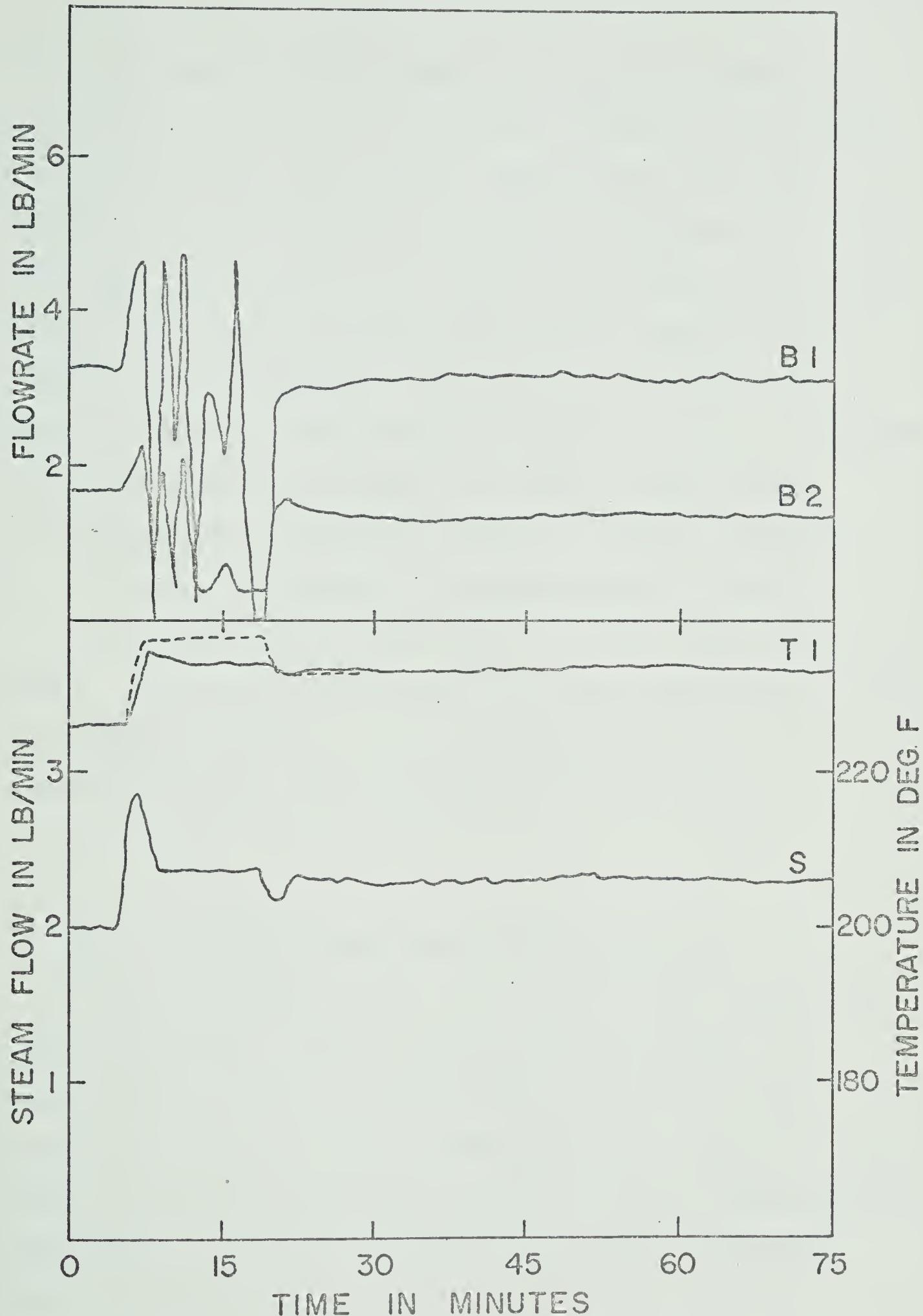


FIGURE 7b: Response of Flow Rates and Temperature for Time Optimal Control
 ——experimental, Model 5LF, --- Model 5LF

curve in Figure 7 is the response of C_2 from Figure 6 replotted for convenience. The model response of T_1 , dashed line in Figure 7b, more closely approximates the process response than in Figure 6b. A similar improvement in the modelling accuracy, model 3, Table 1 was obtained by experimentally "tuning" the second order model, model 2, Table 1, fitted to the theoretical five equation nonlinear model. Model 3 produces a satisfactory process response as indicated by the dotted curve in Figure 6. Model 2 had a large switching error of about ten minutes. This is indicated by the large discrepancy in τ_2 between models 2 and 3.

In general fitted models perform better than theoretical models. The multivariable model could be improved by fitting it to process responses such as those of Figures 6 and 7 instead of to open-loop responses to steam steps.

6.3.2 Control After State Driving ($t > t_f$)

The time optimal policy stops at the time the desired state is reached. Since W_1 and W_2 are not driven to their desired steady states, the regulatory control strategy restores liquid level status. Averaging level control is used normally and as a result the offsets in levels remaining after conclusion of state driving were very slowly eliminated. Refer to Figure 6.

A strategy was devised for more rapid level response whereby the bottom flow rates were set to their predicted steady state value plus or minus the equivalent of proportional action with the specific offset. Figure 8 indicates this technique produces more rapid level response however it has a detrimental affect on the product concentration profile. This indicates that the feedback control used in the product concentration loop is inadequate during large level upsets. An alternative is to drive the levels as well as the product concentration as was done in Chapter Four. An integral criterion which includes the levels is another alternative.

6.4 Selecting a Nominal State for Linearization

Since the point of linearization is arbitrary, the question arises as to which state provides the "best" linear model for derivation of the optimal control policy. Two obvious choices are the initial steady state and the final (desired) steady state. If the initial steady state represents the normal plant operating state then it is an obvious choice. This is particularly true if the changes are never going to exceed the range in which the model linearization is valid and if the model is used for other purposes such as state estimation and/or multivariable regulatory

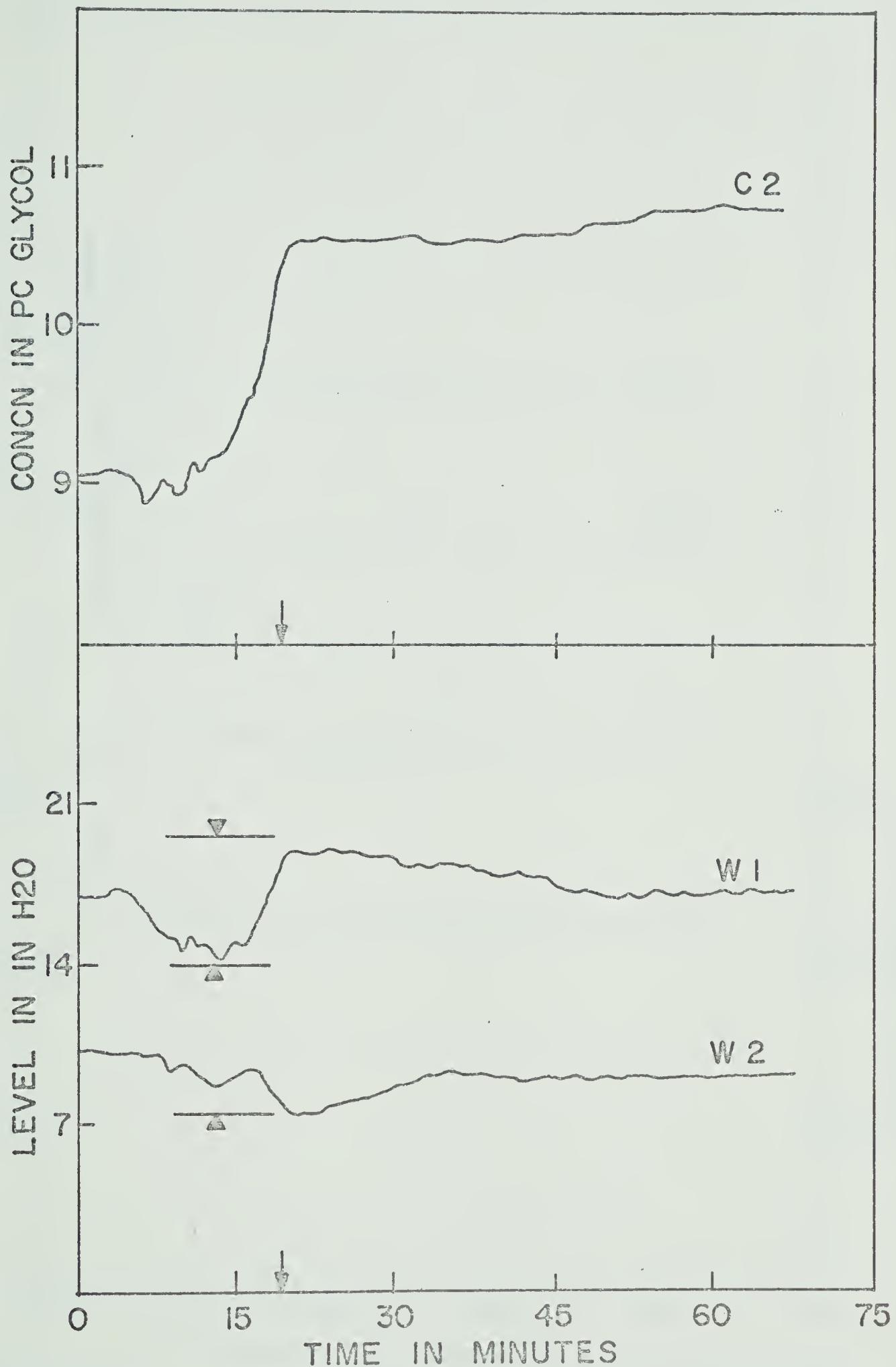


FIGURE 8a: Response of Concentration and Liquid Levels with Fast Liquid Level Recovery $t > t_f$

— experimental, Model 5LF

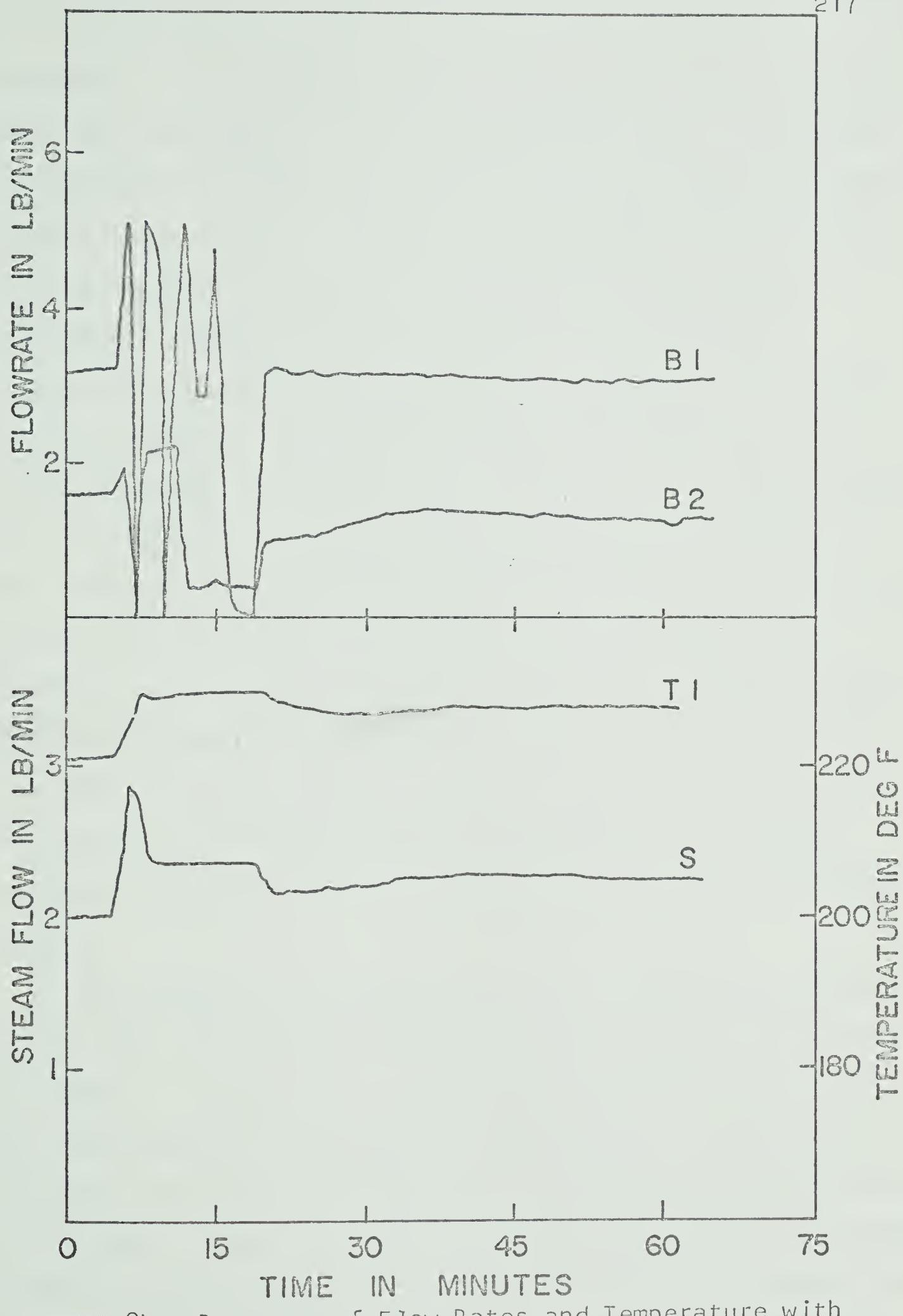


FIGURE 8b: Response of Flow Rates and Temperature with Fast Liquid Level Recovery $t > t_f$

— experimental, Model 5LF

control. If the desired state is to be used then two points must be considered. First this makes the model a function of the desired state and it will have to be recalculated for each process change. Secondly a consistent estimate of all the variables in the model (i.e. all state and control variables) must be available and this state must be a realizable, "equilibrium-point" of the process. (In theory a "controllable" model can be driven to the desired state even though the specified state is not an equilibrium point). Use of the desired steady state does permit the problem to be stated in the usual textbook form of driving an unforced system, with non-zero initial conditions, to the origin. However, since there is seldom any means of picking the best state to linearize about, a priori, it is usually more convenient to use the initial state. If more accuracy is required then fitting the linearized model to the process response over the region of anticipated changes is probably best.

The effect of linearization of the theoretical nonlinear model about the initial versus the final operating condition is shown in Figure 9 for a change of two percent by weight in the setpoint of the product concentration. OS/360 CSMP [18] was used for the simulation of control policies derived from models 5L and 5LD linearized about the initial and final states respectively. The object is to drive the product concentration to the desired setpoint in minimum time while

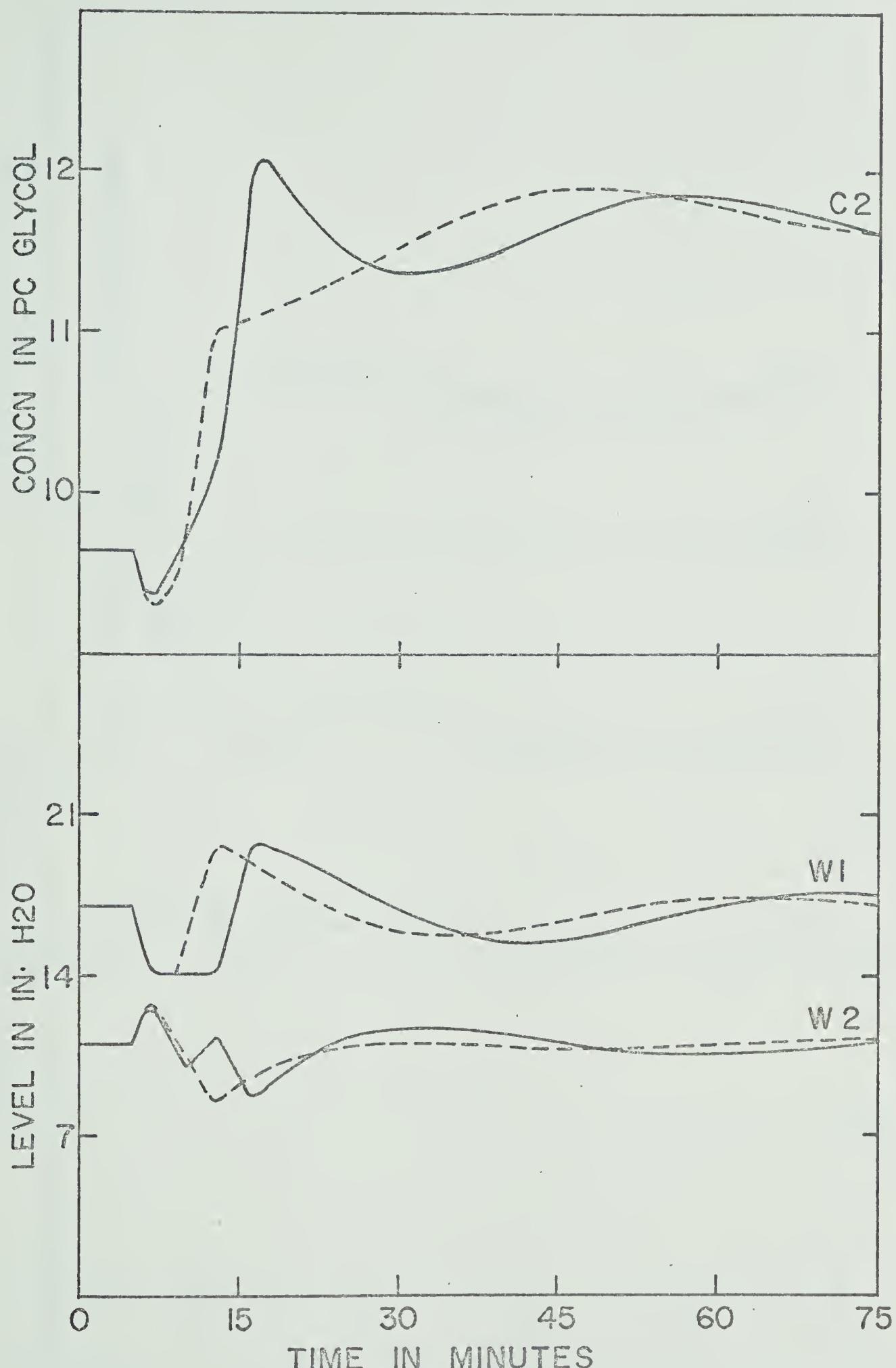


FIGURE 9a: Concentration and Liquid Level Response of Model 5NL to Control Policies Derived from Model 5L (—) and Model 5LD (---)

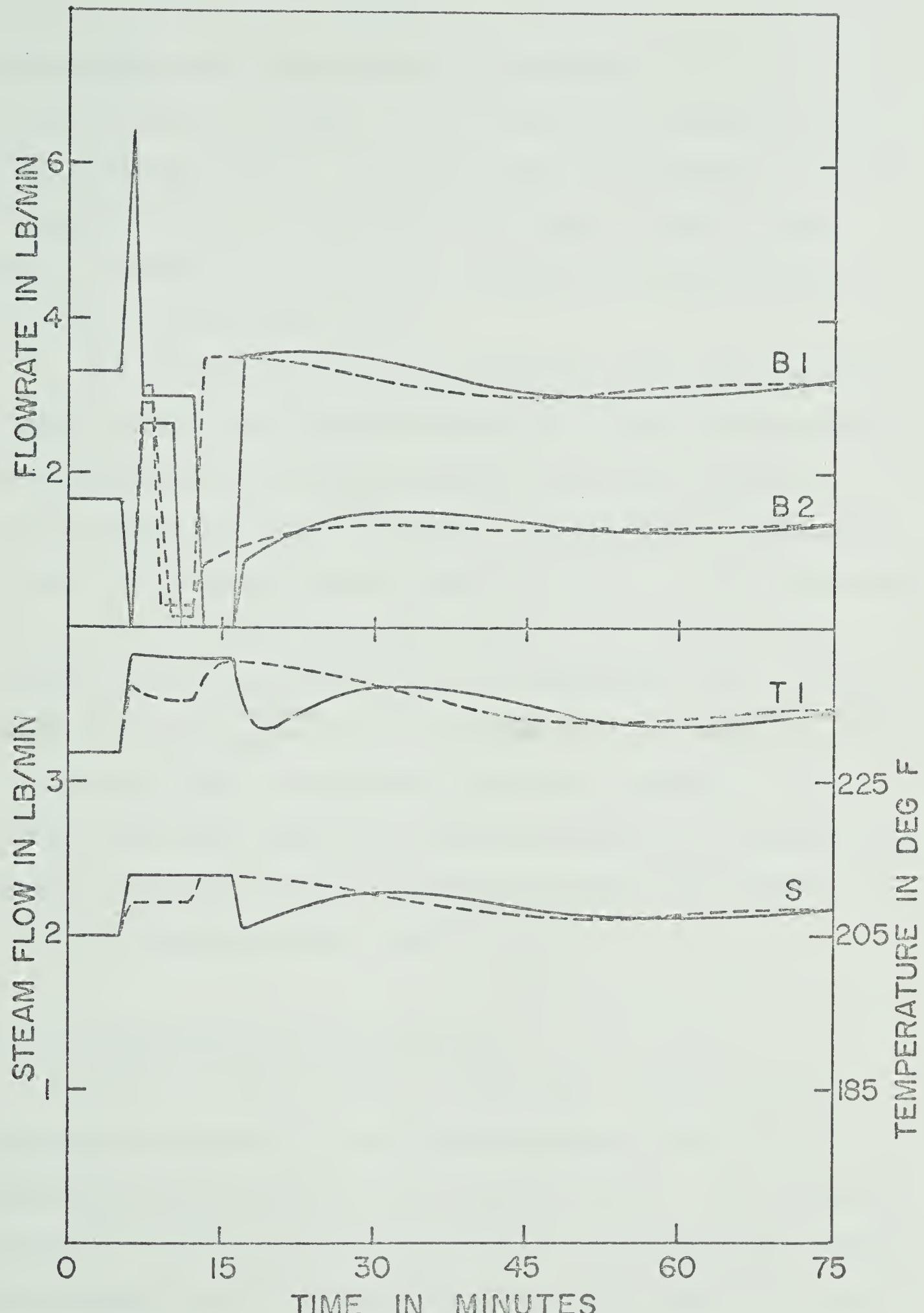


FIGURE 9b: Flow Rates and Temperature Response of Model 5NL to Control Policies Derived from Model 5L (—) and Model 5LD (---)

the holdups are constrained to be within ± 5.0 lb of the nominal process holdups. The first effect temperature is not to exceed 240°F. This constraint is necessary because a safety valve in the first effect vapor space of the unit releases for a pressure in excess of approximately ten pounds per square inch.

The responses in Figure 9 indicate that linearization about the initial condition predicts a lower concentration to steam gain than actually occurs over the transient since some overshoot is evident. Linearization about the final steady state has the opposite effect. This phenomenon is due to the nonlinear gain between concentration and steam which results when water is evaporated from a dilute versus a more concentrated solution. An intermediate steady state would seem to compromise the two responses. This effect was also noted in a previous study which compared the linear evaporator model responses to load disturbances with the actual process response [19].

6.5 Evaluation of SAE Criterion

There is a conspicuous "wrong way" response in the product concentration profiles associated with the time optimal control policies of Figures 7 and 8. This anomaly results from the opposing effects of increased steam versus increased inter-effect bottoms flow. The use of an integral criterion removes this anomaly. The sum of the absolute

errors, SAE, criterion was utilized since it is a popular, linear criterion. The holdups and the first effect temperature (pressure) were constrained. However in order to avoid large level upsets (Figure 8), the levels and the product concentrations were weighted, the product concentration is most heavily.

The response with this criteria is represented graphically in Figure 10. The C_2 profiles in Figure 7 can be compared directly. The time optimal response is more rapid. However, the wrong way response has been removed in Figure 10. The actual process concentration profile (solid) again lagged that of the linear model (dashed) significantly. As expected the control action and the process response to the setpoint change is much less erratic.

The dotted line in Figure 6 is the experimental single loop time optimal response for a corresponding setpoint change. Again increase rate of response is evident in the multivariable case when Figures 6 and 10 are compared.

The SAE criteria produces a more acceptable process response than the time optimal. Further experimental runs with this criterion will be presented in the evaluation of the proposed scheme for addition of this policy to a conventional regulatory control system.

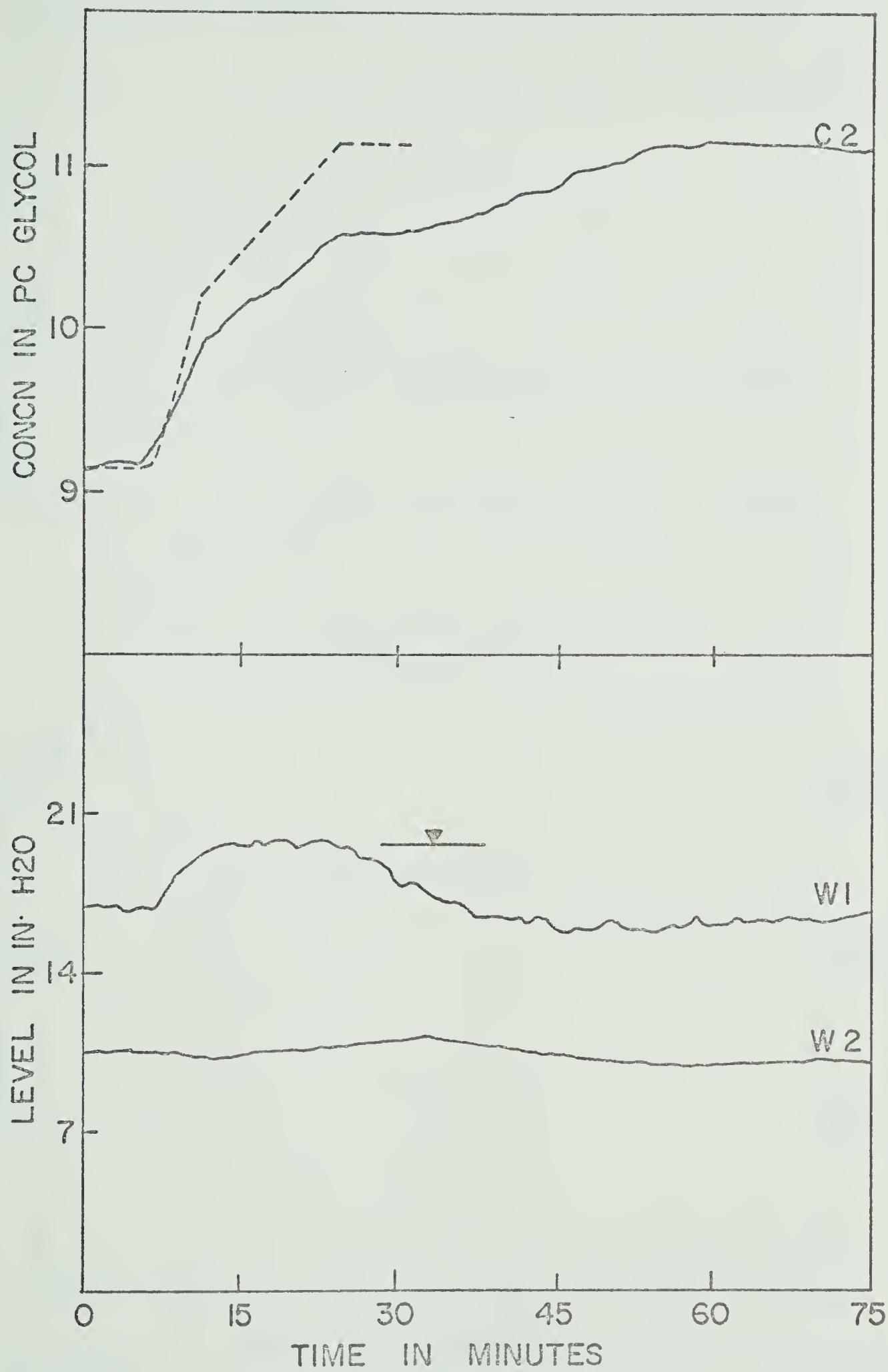


FIGURE 10a: Concentration and Liquid Level Response to Control Based on Model 5LF, SAE Criteria
--- model 5LF, —— experimental

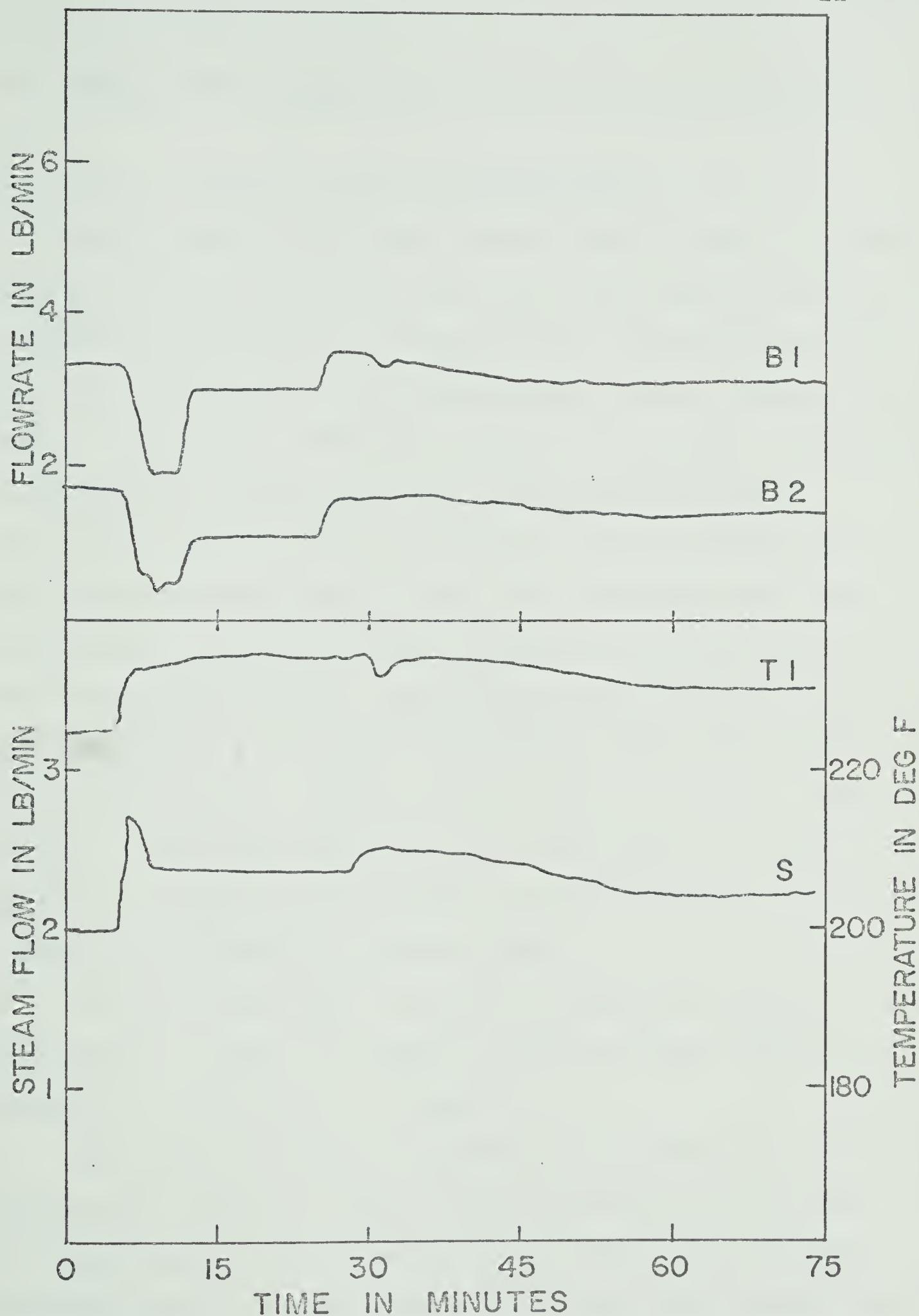


FIGURE 10b: Flow Rate and Temperature Response to Control
Based on Model 5LF

6.6 Comparison of Open Versus Closed Loop Implementation

6.6.1 Single Variable Implementation

Using equation (13) as a control model, analytical time optimal switch times were calculated using a golden search technique as discussed in Chapter Four. Concentration control was maintained by the conventional cascade control loop shown in Figure 5. Discrete values of the optimal concentration profile, $C_2^*(t)$ (predicted using equation (13) as the process model), are put directly into the setpoint of the concentration control loop. The output from the concentration controller is sent directly to the setpoint of the steam control loop. Fortunately the standard DDC algorithm contains provision for adding a bias term so that the optimal control action, $S^*(t)$, could be added to the output of the steam controller as illustrated in Figure 4. Details of the control programs for implementation of this scheme are documented elsewhere [17].

At the final time, the optimal trajectory, $C_2^*(t)$, approaches the desired setpoint and thus normal regulatory control is automatically resumed.

Considering feedback compensation for modelling inaccuracies, Figures 11 and 12 show simulated OS/360 CSMP, and experimental results respectively of programmed state driving based on a "poor" empirical second order model, model 1, Table 1. The solid curves are open loop programmed control

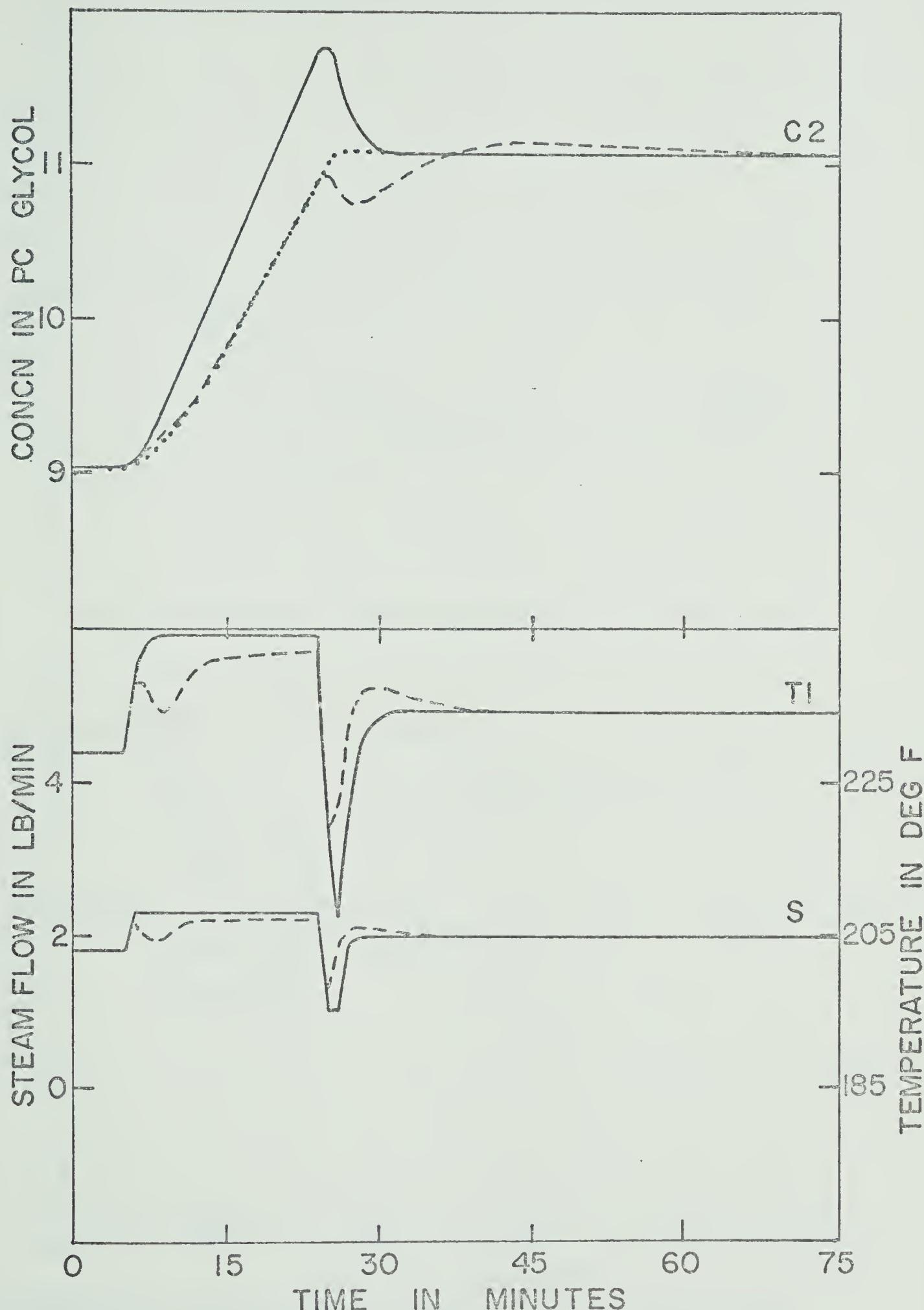


FIGURE 11: Simulated Response to Control Based on Second Order Model 1
 — open-loop, --- closed-loop, ... control model

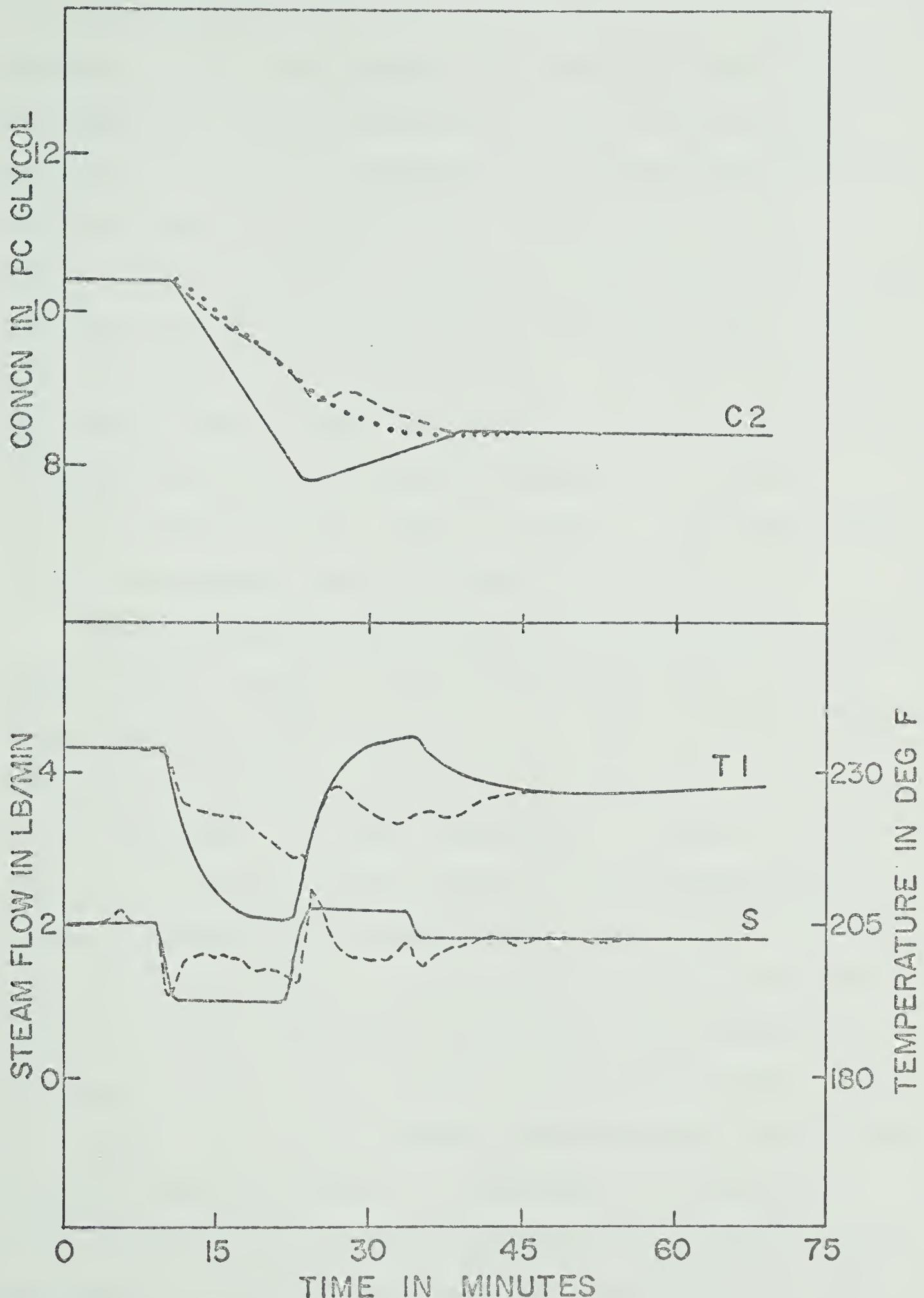


FIGURE 12: Experimental Response to Control Based on Second Order Model 1
 — open-loop, --- closed-loop, ... control model

trajectories while the dashed lines represent the trajectories generated using the same control policy that produced the solid curves but implemented in a closed-loop configuration analogous to Figure 4. The dotted curve is the control model or optimal trajectory. Level loops were placed on tight control and proportional control was used in the product concentration feedback loop. In Figures 11 and 12 the control model "lags" the process. Figure 13 shows the simulated results of a setpoint response for a case in which the control model, model 2, Table 1, leads the process. This is the normal case with theoretical models.

Another cause for poor response during setpoint changes under optimal control is disturbances which have not been accounted for in the control policy. The most severe load disturbance encountered by a control system for this pilot plant evaporator is a feed disturbance. Figure 14 and Figures 15 and 16 show the response of programmed control based on models 2 and 3 respectively. The solid lines indicate the trajectories followed under open loop programmed control with the indicated simultaneous feed disturbance. The dotted line is the response of the control model. The dashed line is the trajectory obtained with the combined control scheme of Figure 4. Improvement is evident for both simulated (Figure 14) and experimental (Figures 15 and 16) results. In both cases the feed disturbance was such as

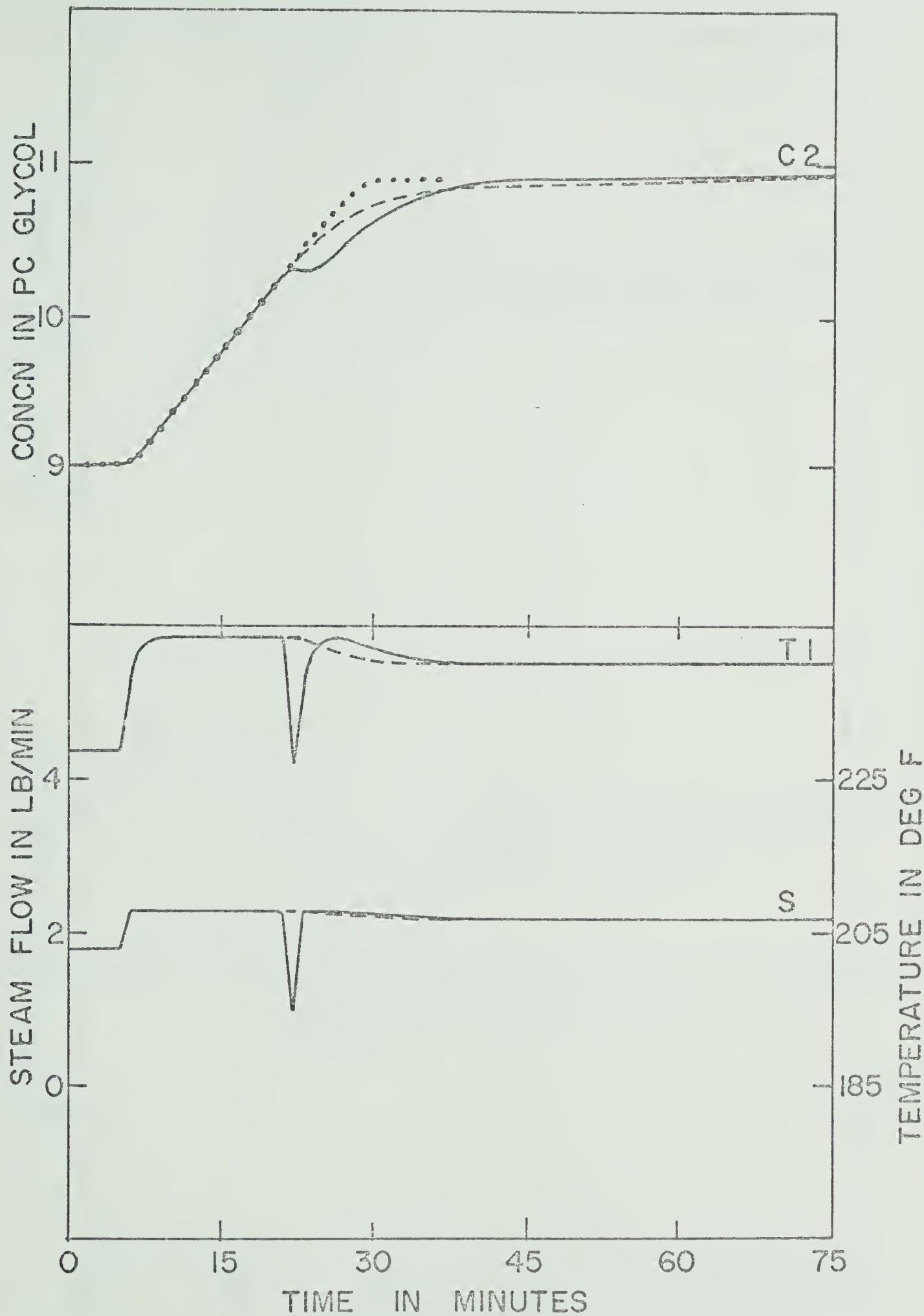


FIGURE 13: Simulated Response to Control Based on Second Order Model 2
 — open-loop, --- closed-loop, ... control model

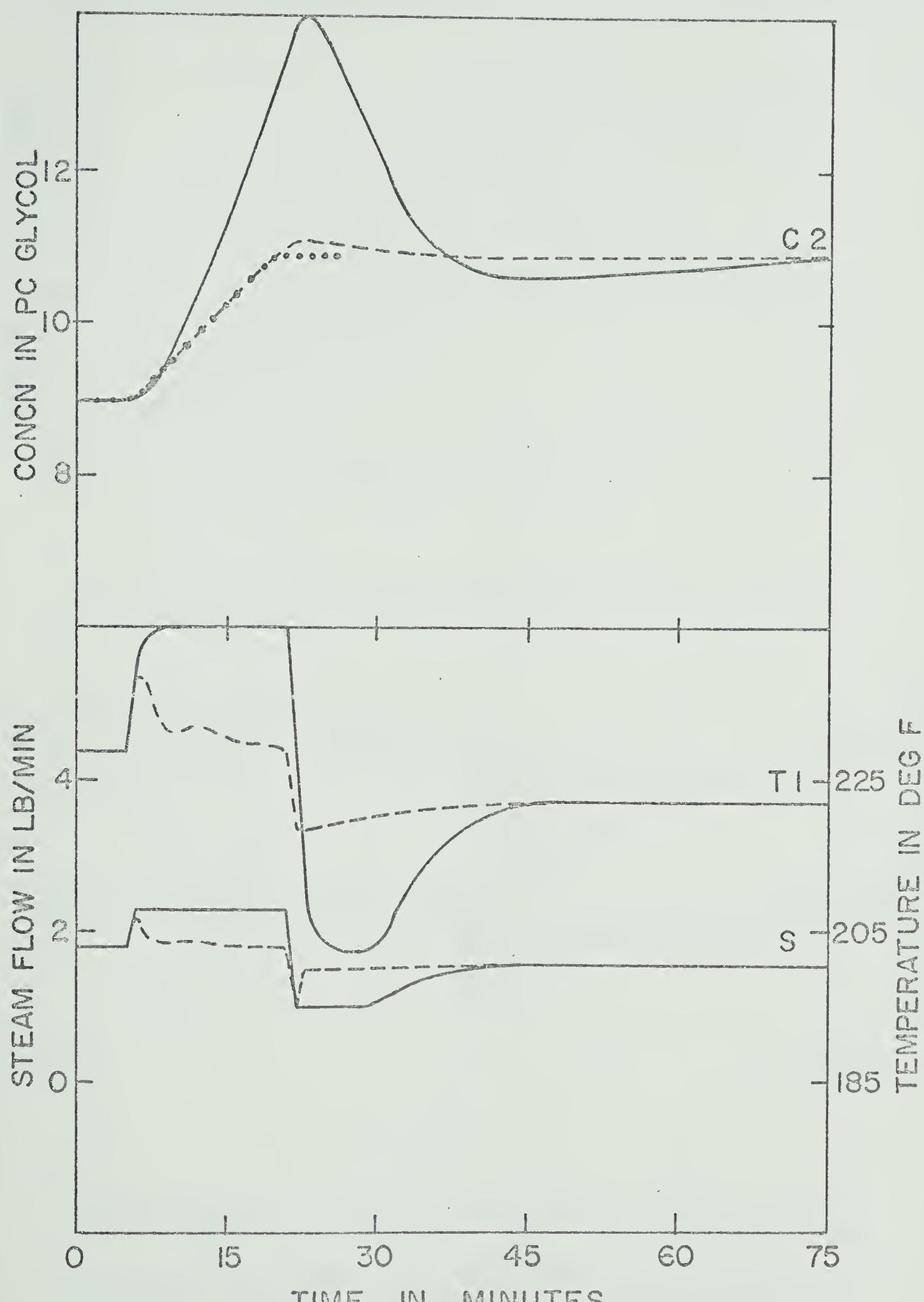


FIGURE 14: Simulated Response to Control Based on Model 2 with (-20%) Feed Disturbance
 — open-loop, --- closed-loop,
 ... control model

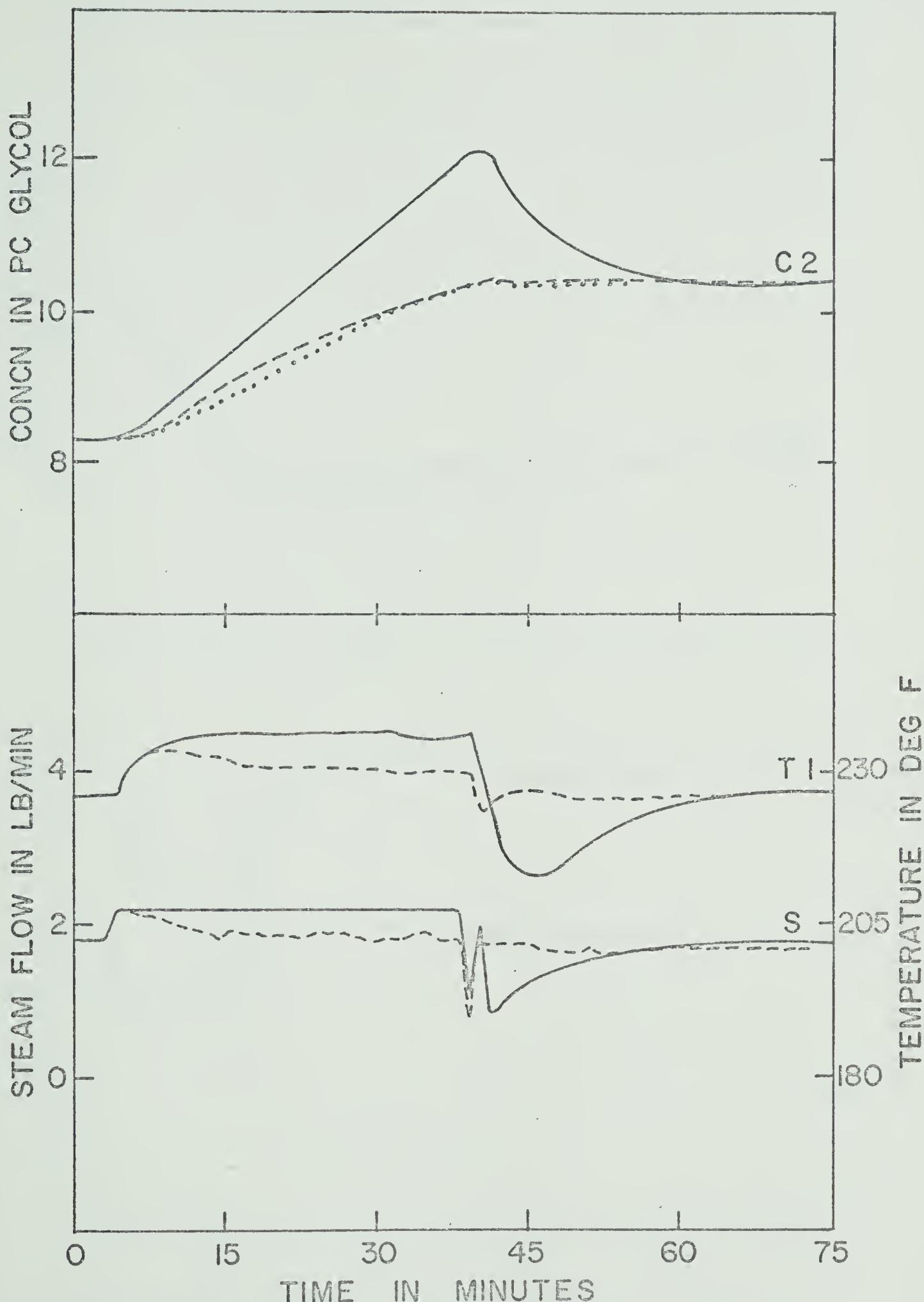


FIGURE 15: Experimental Response to Control Based on Model 3 with (-10%) Feed Disturbance
 — open-loop, --- closed-loop,
 ... control model

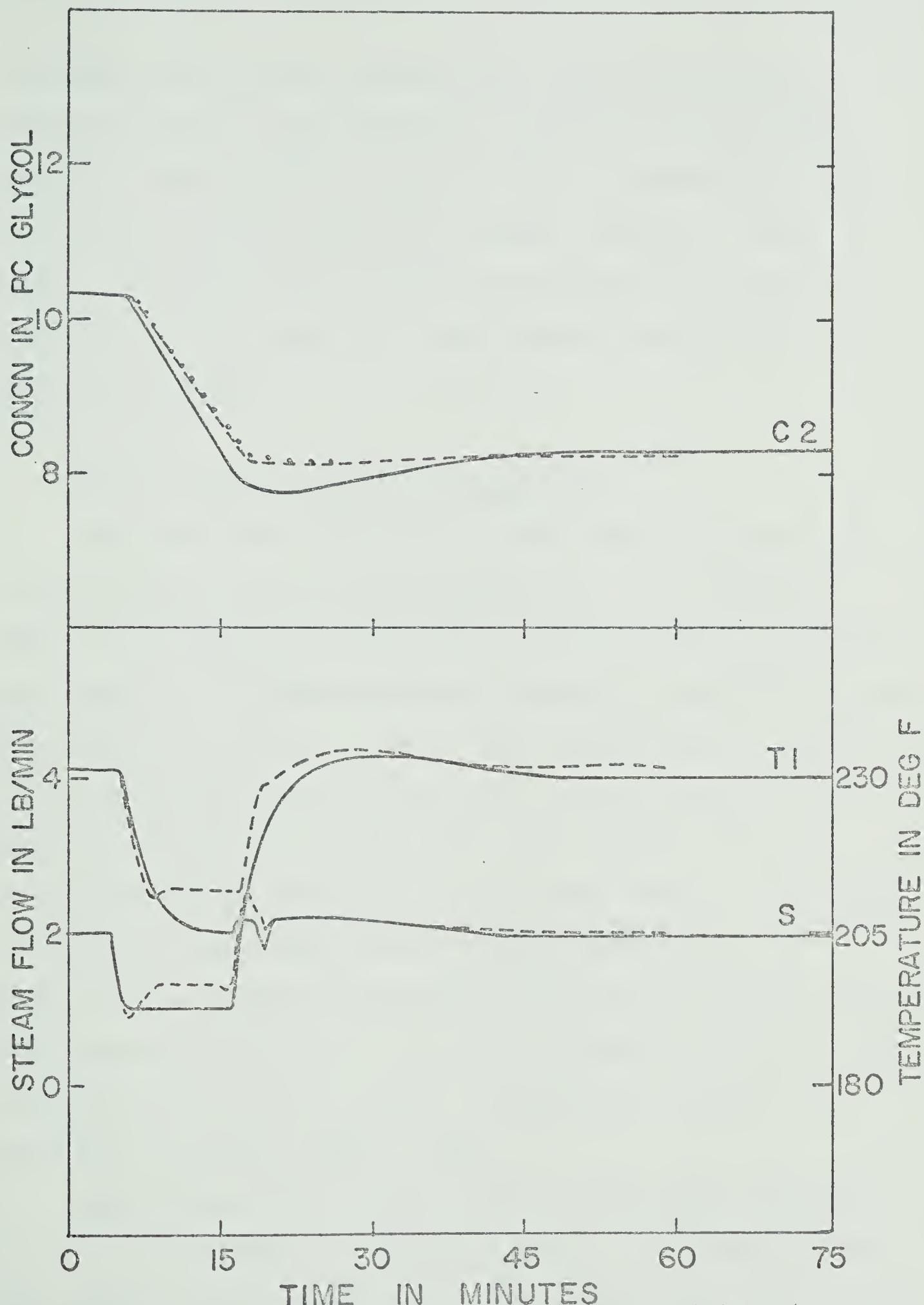


FIGURE 16: Experimental Response to Control Based on Model 3 with (+25%) Feed Disturbance

— open-loop, --- closed-loop, ... control model

to hasten the process response thus causing overshoot. Figure 17 depicts the simulated results of a suboptimal setpoint change based on model 2 with a simultaneous feed disturbance which impedes the process response. Once again, since the time for which the steam is at its lower constraint is so small, the improvement attained with the feedback is small.

6.6.2 Multivariable Implementation

Using the SAE criterion, an open-loop policy was derived from the linear programming algorithm. Figure 18 shows the results of closed loop implementation as defined by Figure 4. The concentration control was achieved in the same manner as for the single loop implementation except $C_2^*(t)$ was predicted by model 5LF. As well optimal level profiles (predicted by the fifth order model) were put directly into the setpoints of the level loops. The output from these loops went directly to the setpoint of the bottoms flow control loops where the open loop control action was introduced into the bias in an analogous fashion to the concentration control scheme. Proportional control was used for all three control loops.

The dotted line on the C_2 plot is the model response, this is the optimal trajectory, $C_2^*(t)$. The dashed line is the closed-loop implementation. No output limit was imposed on the steam, therefore, since the process response lagged the model response, feedback action increased steam and this

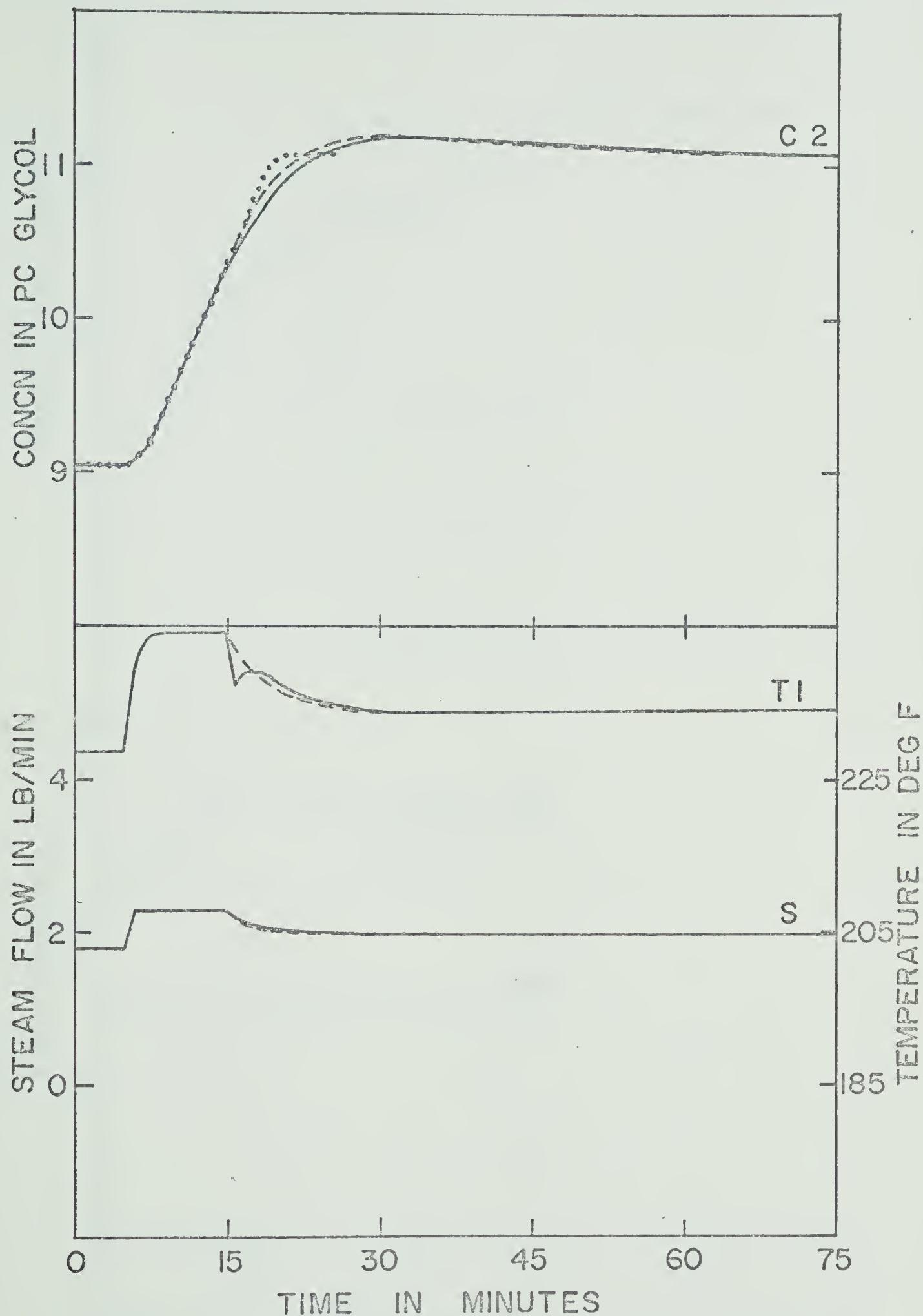


FIGURE 17: Simulated Response to Control Based on Model 2 with (+10%) Feed Disturbance

— open-loop, --- closed loop; ... control model

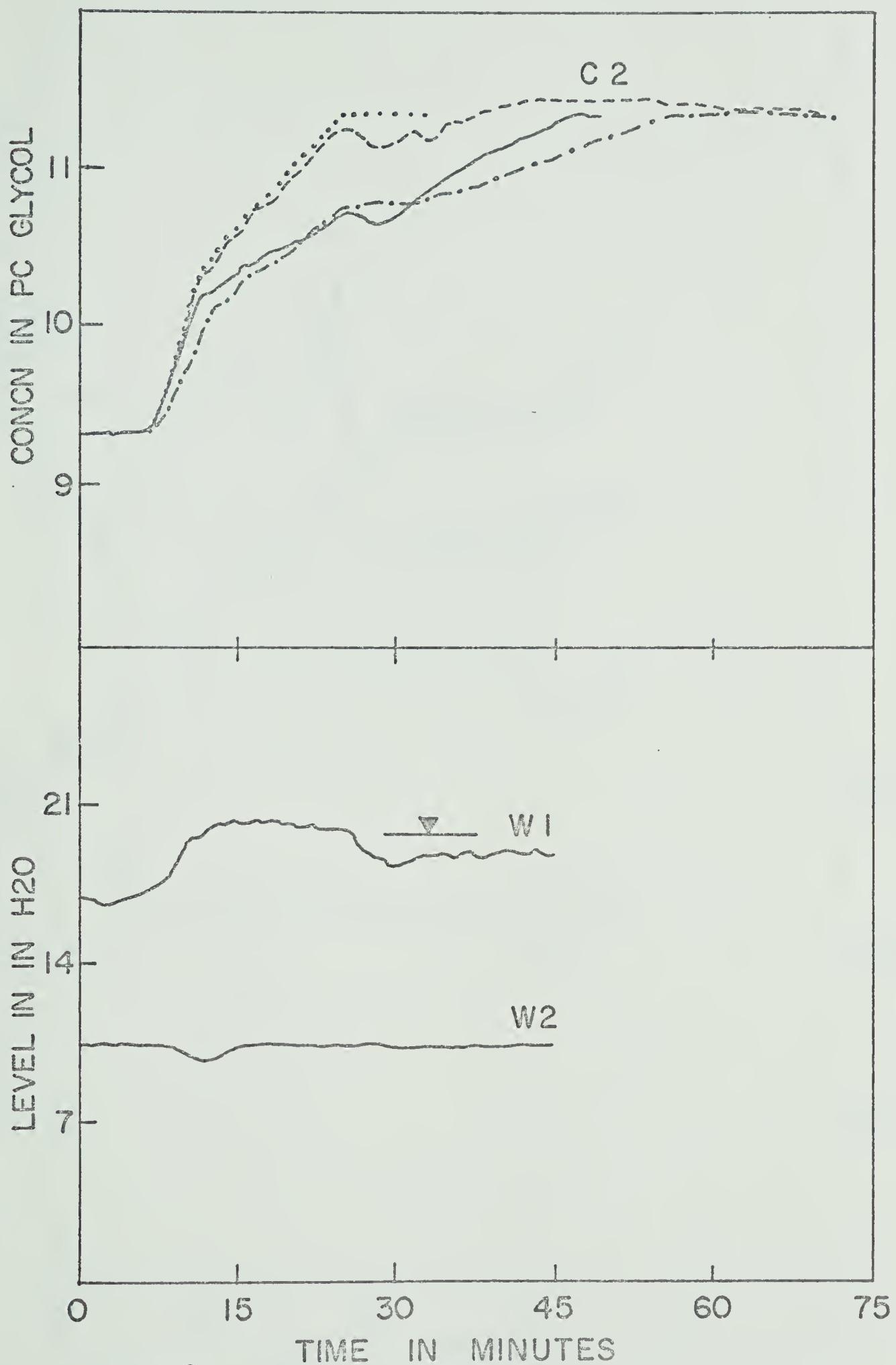


FIGURE 18a: Experimental Response to Control Based on Model 5LF, SAE Criterion
 — open-loop, --- closed-loop, -·- closed-loop (output limit), ... control model

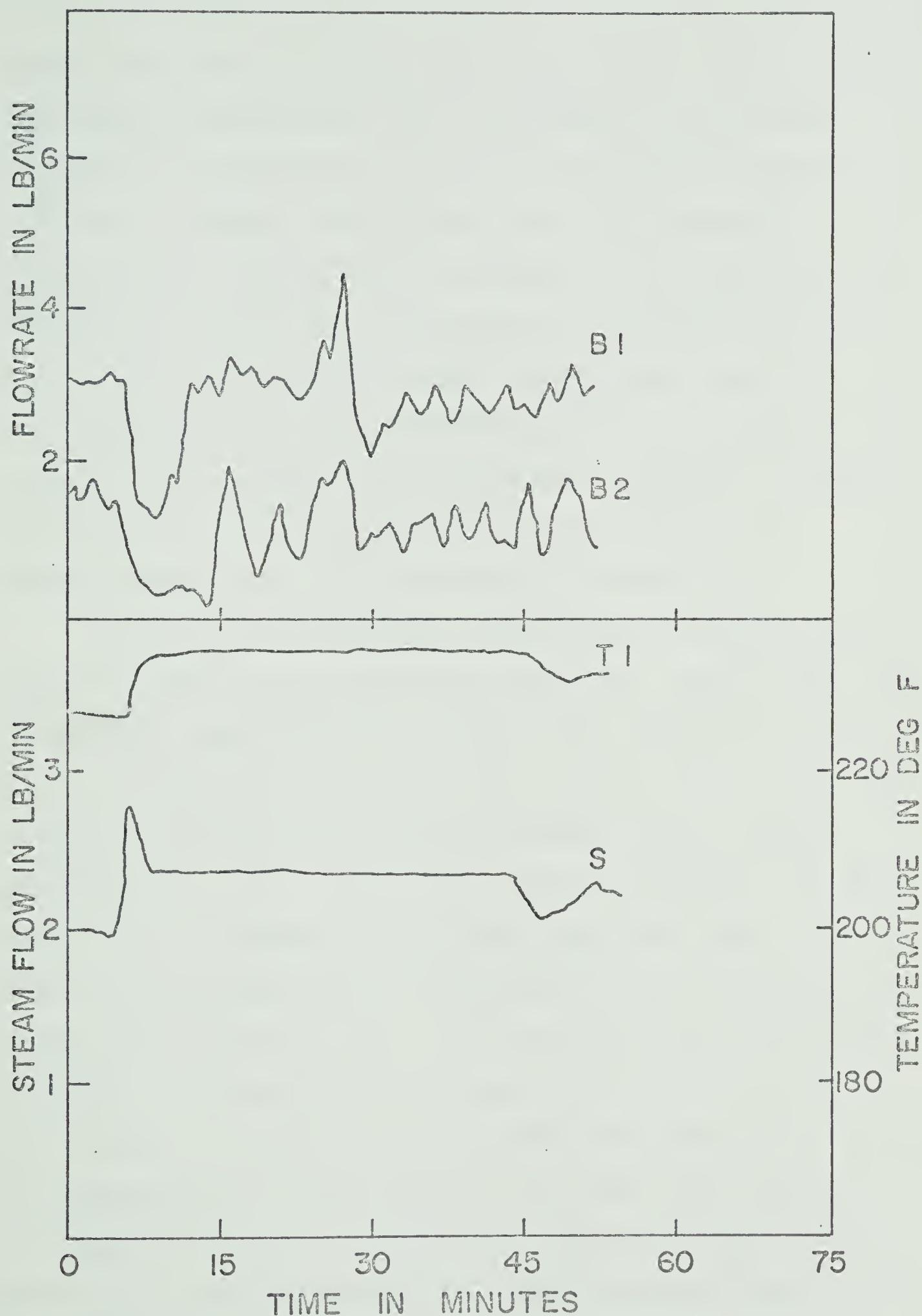


FIGURE 18b: Experimental Response to Control Based on Model 5LF, SAE Criterion
 — open-loop implementation

caused violations of the pressure constraint. The profile does however demonstrate that the feedback action does compensate for modelling errors by following the optimal trajectory closely. The solid curve is an analogous implementation except that the output of the steam loop is limited to a value which maintains an acceptable pressure in the first effect vapor space. Improvement over the corresponding open-loop implementation, the solid curve in Figure 10, is evident. This open-loop response of product concentration has been retraced on Figure 18 as the dashed-dotted curve for convenience of comparison.

Figure 19 is an analogous experimental response for a setpoint change in the opposite direction. Notice that the closed loop implementation (dashed line) resulted in overshoot of the product concentration. This resulted from the interaction of the first effect bottoms and the product concentration. The first effect level is difficult to predict in this instance. The actual level was higher than predicted causing feedback compensation which increased the first effect bottoms flow. It is evident that a multivariable feedback system would perform much better than the multi-loop system of Figure 5 in this case since interactions would be compensated for more rapidly. The open loop response is represented by the solid line. Again the dotted plot depicts the optimal trajectory (i.e. the control model response). A lower limit was placed on the first effect

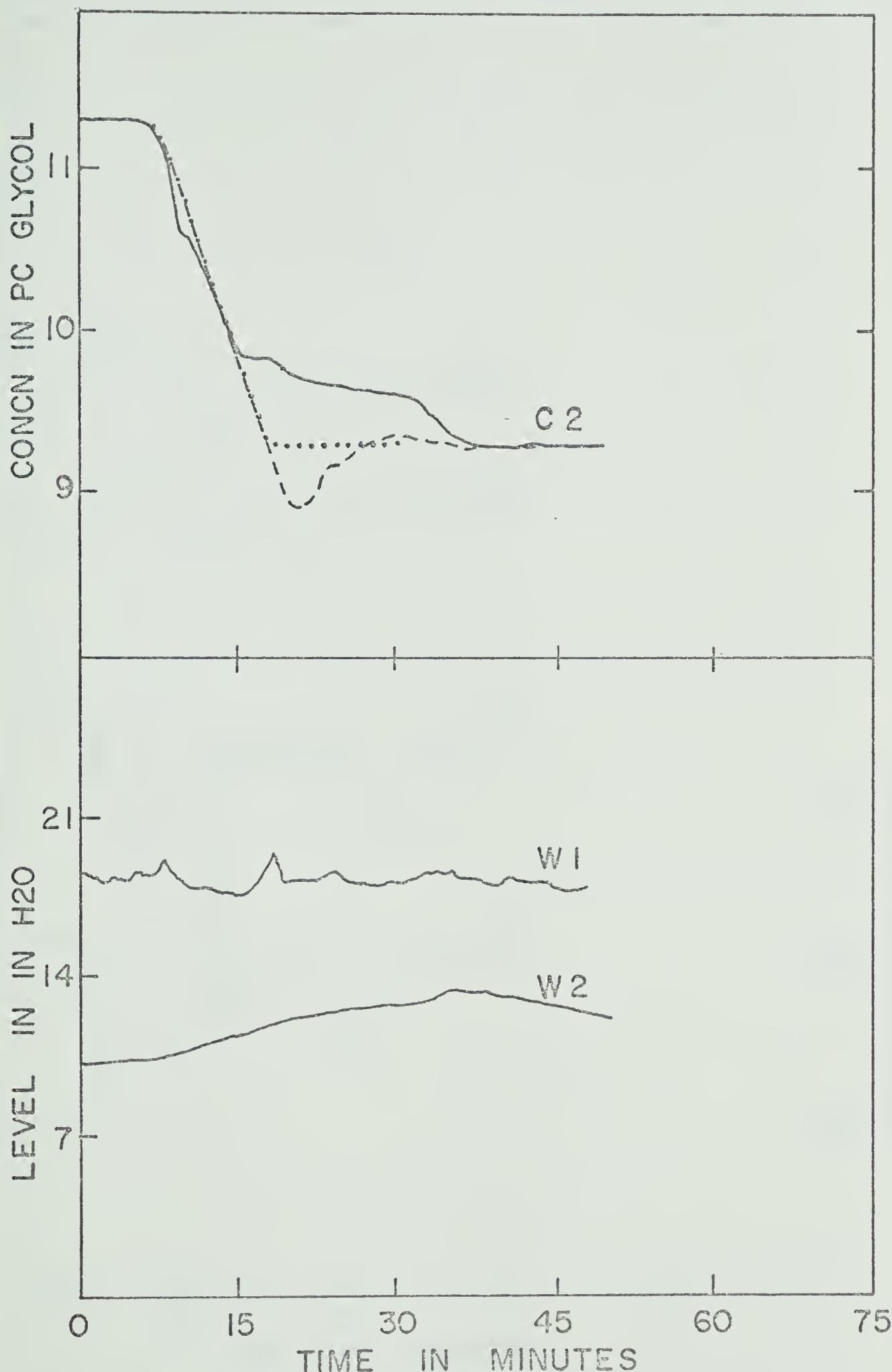


FIGURE 19a: Experimental Response to Control Based on
Model 5LF, SAE Criterion
— open-loop, --- closed-loop,
... control model

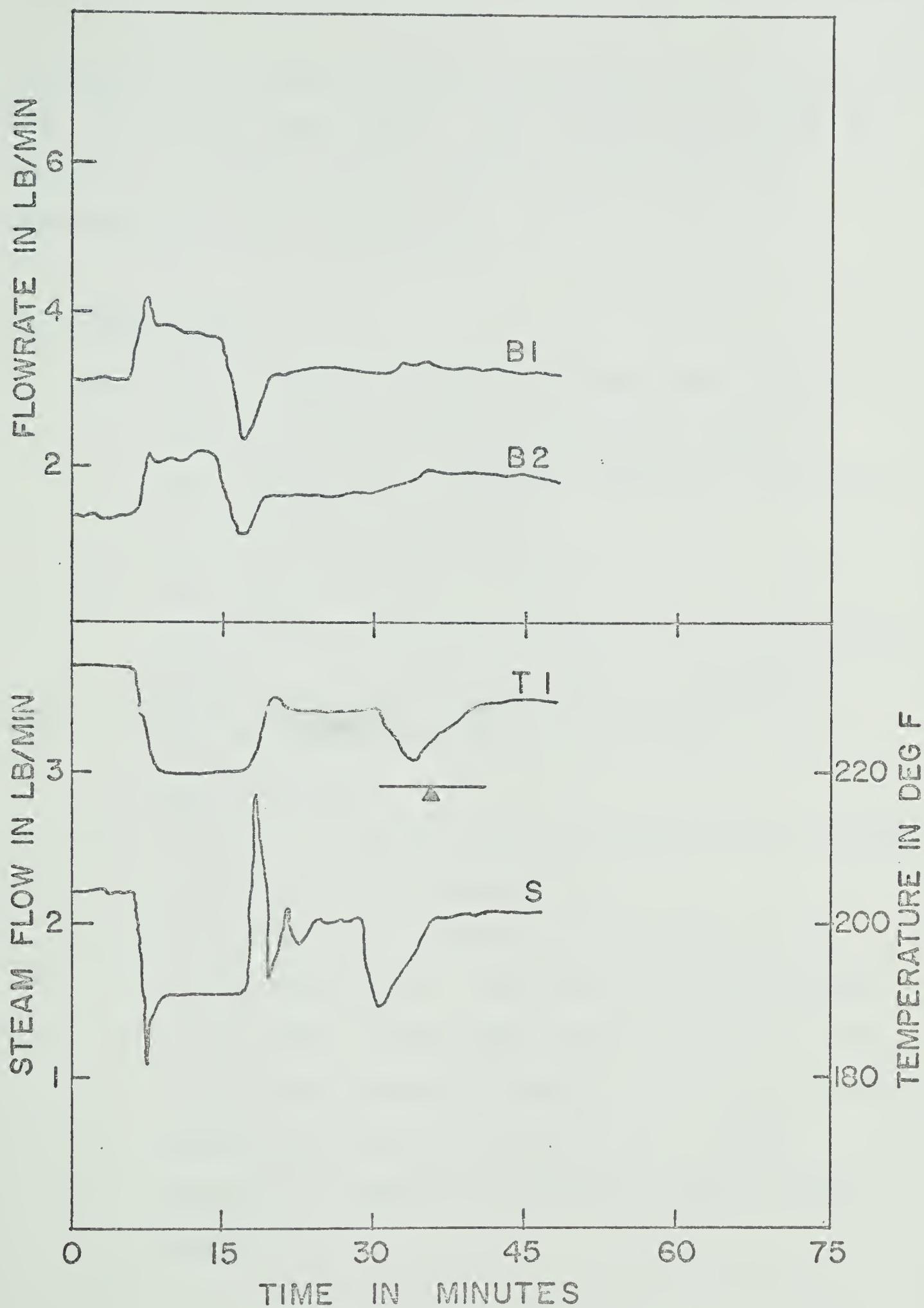


FIGURE 19b: Experimental Response to Control Based on Model 5LF, SAE Criterion
— open-loop implementation

temperature (pressure) so that a vacuum was not created in the first effect vapor space. This explains the spike in the steam trajectory (solid curve) for the open loop implementation, see Figure 19b.

7. CONCLUSIONS

1. Optimal state driving techniques under manual or computer control produced improved responses over conventional setpoint regulatory control on a pilot plant evaporator.
2. The linear programming formulation is flexible and permits constraints on both control and state vectors. The process engineer is, therefore, able to tailor the response to his desired specifications.
3. Different criteria result in dramatically different process transient responses.
4. Fitted models in general perform better than theoretical models. The point of linearization of the model affects the control policy but the initial conditions are the most convenient steady state conditions for linearization. Model accuracy is important in optimal control implementation.

5. The interface of programmed setpoint control to a conventional control scheme presented in this work is convenient computationally as well as in implementation. This suboptimal control scheme at least partially compensated for modelling errors and load disturbances.
6. Multivariable process models proved to be superior to low order models since they accounted for interactions and permitted constraints to be specified on additional variables.
7. Many practical problems in data reduction and processing, optimization and implementation arise during the synthesis of optimal control policies for real processes.

CHAPTER SIX

AN INTUITIVE APPROACH TO THE SUB-OPTIMAL
CONTROL OF NONLINEAR SYSTEMSABSTRACT

Computation of sub-optimal controls of nonlinear systems using a parameter estimation algorithm in which the parameters in an assumed functional representation of the control variables are calculated, is performed using only the state equations. The method is more intuitive than rigorous optimization methods. Separation of the control policy from the control model allows consideration of higher order dynamics and state constraints which are often neglected in reduced control models. Simulated results from a fifth order nonlinear evaporator model are used to emphasize the advantages and demonstrate the approach.

1. INTRODUCTION

In certain situations a linearized model does not adequately represent the process dynamics of a nonlinear system. Either a series of linear models or a rigorous nonlinear model is required to describe the process dynamics. Implementation of control policies derived from a "chain" of linear models is difficult due to the problem of matching states.

This chapter describes a sub-optimal method of synthesizing a control policy based on a nonlinear model. The technique involves specification of the functional form of the control policy. The unknown parameters in this function are then calculated so as to optimize a performance index which is a function of the model trajectory.

The control policy may be constructed in such a manner as to trade off control complexity versus marginal improvements in minimization of the index of performance. In many cases the form of the optimal control law can be predicted from Pontryagin's Maximum Principle. Time optimal control laws often fall into this category. When the functional form of the optimal control policy is known, the result of the algorithm presented in this work will be optimal, except for errors in numerical solution.

Separation of the control policy from the model order is desirable in many instances due to state constraints and

higher order dynamics which cannot be incorporated into reduced models but can be considered with the rigorous model. For example recall that the reduced second order models of Chapter Four did not include the state constraints and therefore the control law was simpler in its form. Results presented in Chapter Five indicate that model accuracy is important for open-loop implementation of optimal control policies. The sub-optimal control approach presented in subsequent sections is intuitive and is readily "tuned" to the actual process. The computational algorithm employed to determine the suboptimal control policy was developed for parameter estimation as described in Chapter Three. The algorithm employs quasilinearization in conjunction with linear programming.

Computation of the sub-optimal control policy for a model of a pilot plant evaporator, which is composed of five nonlinear differential equations, is used to demonstrate the approach.

2. DEVELOPMENT

Many nonlinear dynamic systems can be conveniently represented by the following vector differential equation:

$$\dot{\underline{x}}(t) = \underline{f}(\underline{x}(t), \underline{u}(t)) \quad (1)$$

with the initial conditions vector:

$$\underline{x}(t_0) = \underline{x}_0 \quad (2)$$

The optimal control problem is to determine the control, $\underline{u}(t)$, which will minimize the following objective function and remain within the bounds $\underline{\alpha} \leq \underline{u}(t) \leq \underline{\beta}$:

$$J = \int_{t_0}^{t_f} L [\underline{x}(t), \underline{u}(t)] dt \quad (3)$$

Constraints on elements of the state vector are also common. Two approaches to the solution of this problem have received the most attention, dynamic programming and Pontryagin's Maximum Principle [1]. The curse of dimensionality prevents the use of dynamic programming for many practical problems. The latter approach leads to the classical nonlinear two point boundary value problem which requires solution by direct iteration, search techniques, quasilinearization or invariant imbedding. However, state and control variable constraints are introduced only with great difficulty. The use of penalty functions for the incorporation of state constraints is popular [2]. Also the numerical integration of the costate equations which arise from Pontryagin's

Maximum Principle are inherently unstable and often are a stumbling block in the way of a practical solution [2].

The approach adopted in this work is to calculate a "sub-optimal" control law in such a way as to avoid the costate equations while allowing easy incorporation of state and/or control constraints into the problem. The optimal control problem is converted into a parameter estimation problem in the following manner. It is assumed that $\underline{u}(t)$ can be represented by:

$$u_i(t) = \phi_i(\underline{a}_i, t) \quad \text{for } i = 1, 2, \dots, m \quad (4)$$

where the vectors \underline{a}_i are vectors of unknown parameters in the functions ϕ_i . These parameters could be coefficients in a polynomial in t , switching times or arguments of transcendental functions. The sub-optimal control problem then becomes one of determining the unknown parameters in the functions ϕ_i such that the objective function, J_1 , is minimized where J_1 is of the form:

$$J_1 = \int_{t_0}^{t_f} \theta(\underline{x}(t), \underline{x}_d) dt \quad (5)$$

or in the discrete form which is more convenient for digital computer solution:

$$J_1 = \sum_{k=1}^N \theta(\underline{x}(t_k), \underline{x}_d) \quad (6)$$

The algorithm employed restricts the objective function represented by equation (6) to a linear or quadratic criterion such as:

$$\text{SAE: } J_1 = \sum_{k=1}^N \underline{q}^T(t_k) |\underline{x}(t_k) - \underline{x}_d| \quad (7)$$

$$\text{Least Squares: } J_1 = \sum_{k=1}^N (\underline{x}(t_k) - \underline{x}_d)^T \underline{Q}(t_k) (\underline{x}(t_k) - \underline{x}_d) \quad (8)$$

Time Optimal: $J_1 = \lambda$ where $\lambda \geq |x_i(t_k) - \underline{x}_{di}|$ for $i = 1, 2, \dots, n$, where J_1 must be minimized for each trial of N.

Other criteria such as minimum rise time subject to a specified settle out time are also possible.

The specific algorithm used in this work requires an initial guess for the unknown parameter values. Quasilinearization is then used to create a linear boundary value problem which is solved by Runge Kutta integration. The ensuing linear estimation which must be solved to obtain new values for the parameters is performed by linear programming methods. Details of the algorithm were presented in Chapter Three.

Davison and Manro [3] using Rosenbrock's hillclimbing method with numerical integration procedures treat the time optimal control problem in an analogous fashion to this work. They present several multivariable numerical examples which however have scalar control vectors. Pollard and Sargent [4] employ the Fletcher-Powell conjugate direction method to calculate time-optimal switch times for a nonlinear model of a binary distillation column. Baily [5], O'Kelly [6] and deRooy [7] describe the techniques which involve assuming the functional form of the control law for determining sub-optimal control policies for linear multidimensional systems.

3. COMPUTATIONAL ASPECTS

During the application of the parameter estimation scheme to numerical examples several computational difficulties were encountered. In general the technique is restricted to a small number of parameters which hampers its usefulness with multivariable systems. The solutions are usually very sensitive to the state variable weighting chosen for the problem.

When calculating bang-bang type control policies involving unknown switching times, state variable trajectories are very sensitive to changes in these switching times. Because linearization is employed in this approach the magnitude of the changes must be restricted. The constrained

parameter convergence technique introduced in Chapter Three is very useful in this context. However, unless the initial guesses for the parameters are very close to the optimal values, the algorithm results in large computation times in order that numerical stability be ensured.

A very desirable feature, which was not implemented in this work, is the adjustment of the integration interval to exactly coincide with the current switching times.

If the number of switch times chosen to characterize the particular bang-bang control law is too large, small switch intervals are obtained [3] and they can be eliminated. By iteration, the user can determine the best specification of the number of switching times for each variable.

4. A NON-LINEAR NUMERICAL EXAMPLE

Consider the nonlinear system:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1-2x_1^2 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u(t) \quad (10)$$

where $|u(t)| \leq 1$. The control variable, $u(t)$, is manipulated in a bang-bang control fashion with three switch intervals and the criterion is minimum time. Table 1 compares the results obtained by Davison and Monro [3] with those obtained in this work. Computational time was approximately 10 seconds on an IBM 360/67 digital computer.

TABLE 1

TIME OPTIMAL SWITCH TIMES

	Initial State		Switch Time		
	x_1	x_2	T_1	T_2	T_3
This Work	1.0	1.0	0.25	2.54	3.06
Davison and Monro [3]	1.0	1.0	0.26	2.52	3.06

5. APPLICATION TO A DOUBLE EFFECT EVAPORATOR

The parameter estimation algorithm was successfully applied to the characterization of several assumed control laws. The criterion employed was that of minimizing the rise time subject to specified limits on the overshoot.

5.1 Description of Process

The pilot plant process is described in Appendix A and the fifth order nonlinear model is summarized in Appendix B. The variable of prime interest is the product concentration which is controlled by manipulation of the steam flow rate. Two other control variables of interest are the liquid levels of the two effects. In this treatment the object will be to obtain rapid product concentration response without violating the upper limit on the pressure (temperature) in the first effect vapour space.

5.2 Conventional Control Law

Attempts to optimize the proportional and integral controller constants of the steam to product concentration loop for set-point changes on a fifth order linear analog computer model were fruitless. The constants could be increased to values which were far too high for stability. The nonlinear five equation model described

in Appendix B was therefore used along with the parameter estimation routine which optimized the controller constants. The dotted curve in Figure 1 depicts the optimal trajectory obtained ($K_p = 0.543$, $K_I = 1.51$). The control law is of the form:

$$u(t) = K_p (c_2 - c_{2d}) + K_I (x_6) \quad (11)$$

where x_6 is a variable which is appended to the state vector. The following differential equation is added to the vector differential equation (1):

$$\dot{x}_6 = (c_2 - c_{2d}) \quad (12)$$

Thus the system is represented by:

$$\dot{\underline{z}} = \underline{f}(\underline{z}, K_p, K_I) \quad (13)$$

The object of the parameter estimation is to chose K_p and K_I such that some function of the difference between the model, equation (13) and the desired product concentration profile is minimized. In this example, a step was chosen as the desired response.

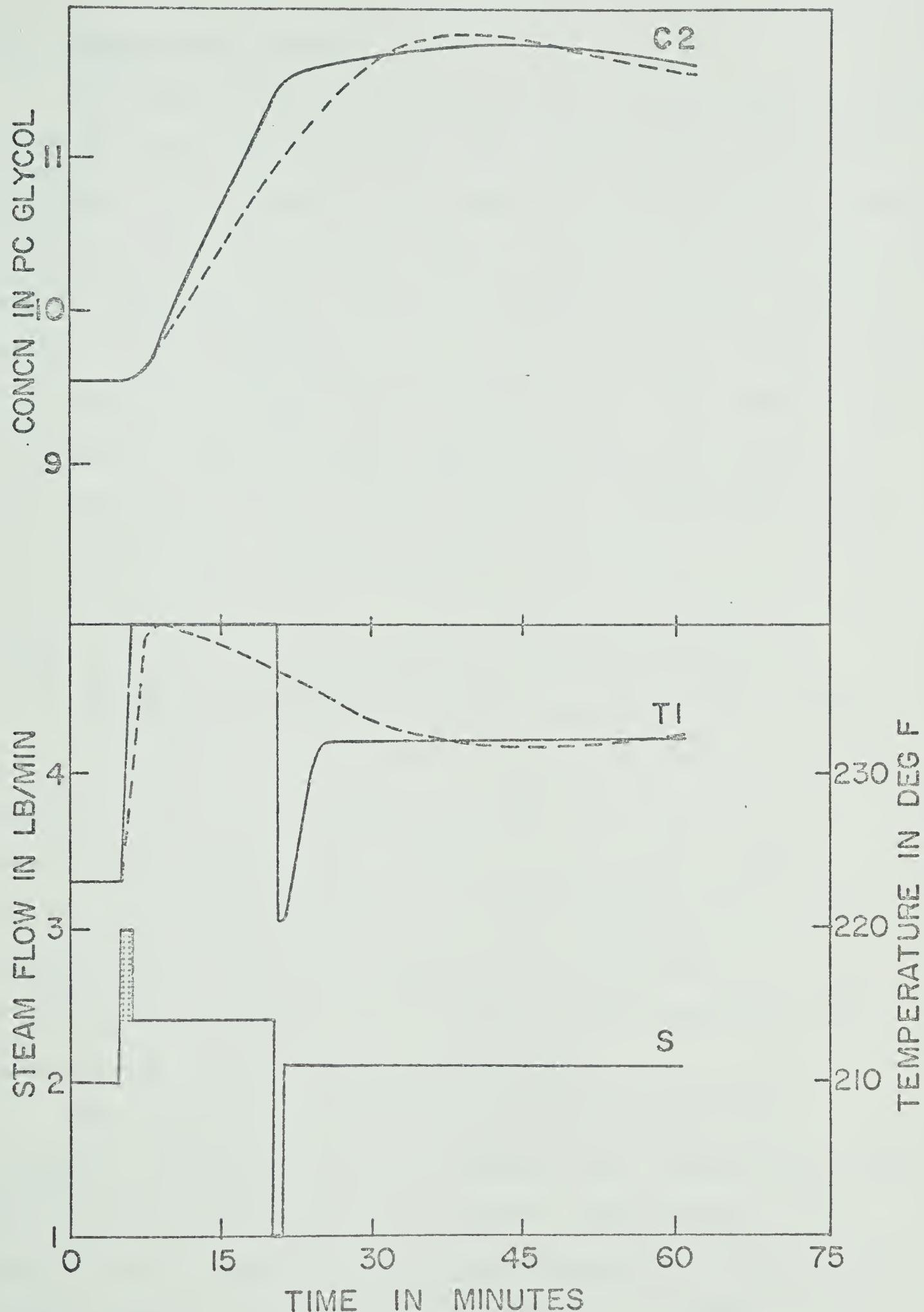


FIGURE 1: Response of Model 5NL to Suboptimal Control Strategies

5.3 Sub-Optimal Control

In Chapter Four it was noted that a second order transfer function model did not account for interactions, constraints or higher order dynamics. By separating the control strategy from the order of the model these "higher" order characteristics may be retained. For a positive change in product concentration a control strategy like the one represented schematically in Figure 2 was chosen for the steam rate. The shaded area in Figure 2 represents the added control action gained over the bang-bang control law derived from a second order model. The second order approach required specification of maximum and minimum steam rates. These values had to be chosen by trial and error so as to conform to state constraints.

The unknown parameters of the control law were chosen to be the three switch times, t_1 , t_2 and t_3 , as well as the magnitudes of the intermediate steps, Δ_1 and Δ_2 . The maximum and minimum steam rates are, of course, known. These constants were chosen so as to minimize the product concentration rise time subject to the constraint of the first effect pressure and to limits on the overshoot and undershoot of the product concentration.

The simulated result is shown as the solid line in Figure 1. Note the improved response over conventional control tuned for servomechanism control applications. The control policy could easily be experimentally "tuned" to the actual process in the same manner that the control policy of the second order models were tuned in Chapter Four.

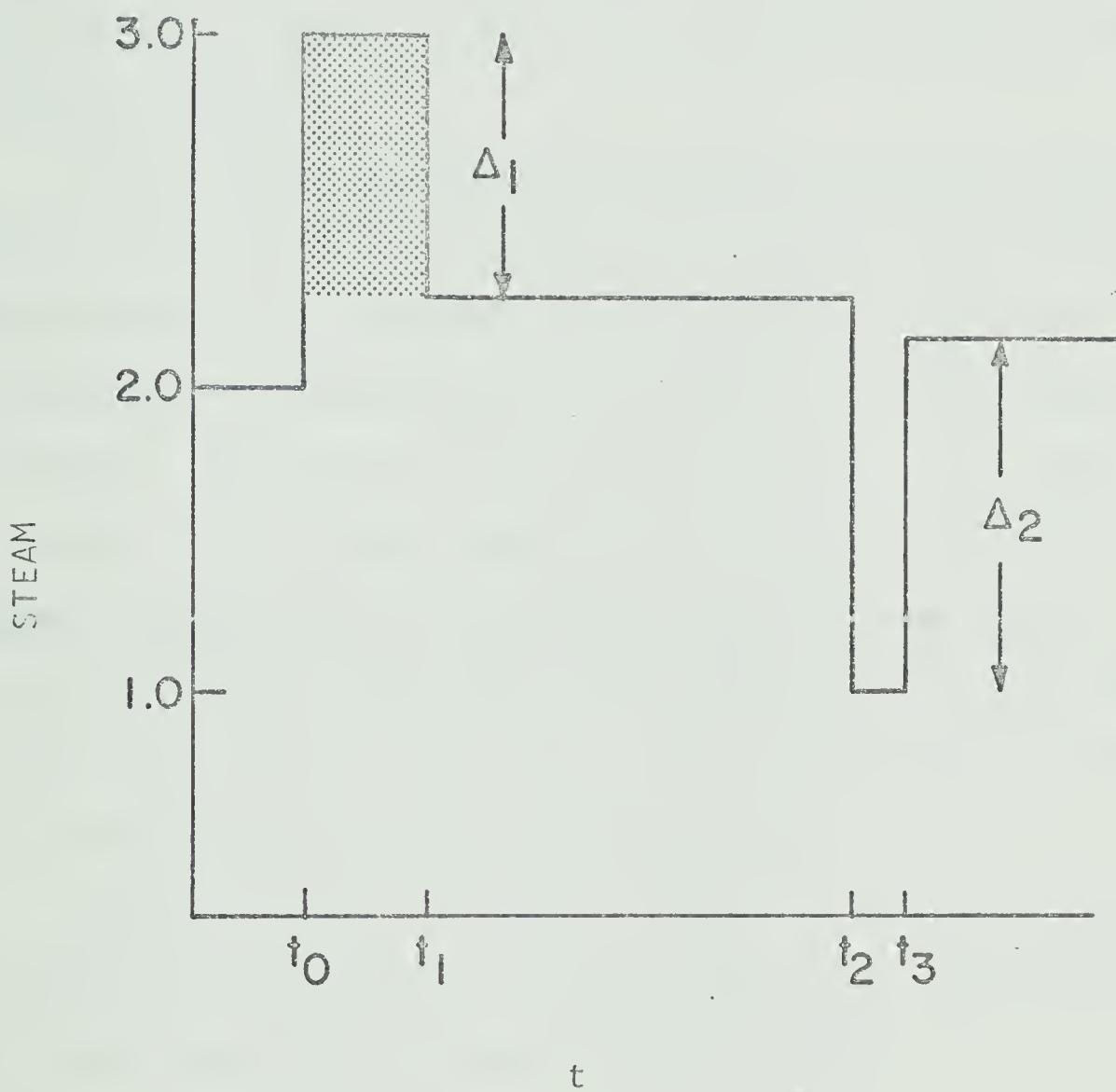


FIGURE 2: Assumed Control Law for Steam

5.4 Startup

During startup of the evaporator the product refractometer reading is unreliable and the vacuum in the second effect is not constant; therefore, if startup is to be optimized, it must be done in an open-loop fashion based on a process model.

The problem considered in this section was to drive the evaporator from a condition in which only levels had been established to the desired operating condition. The object was to minimize the rise time of the product concentration. Again the first effect pressure limit must be imposed. The process model had to be modified over the initial trajectory to include the second effect energy balance until operating temperature was obtained at which time the model reverted to model 5NL. The control vector includes the steam flow rate and the feed rate.

A control law for steam similar to that of Figure 2 was assumed (except $S = 0$ until time t_0). The control law for the feed flow rate was assumed to be:

$$F = 1.0 + 3.5 (1 - \exp(-\lambda t)) \quad (14)$$

It remained to determine Δ_1 , Δ_2 , t_1 , t_2 , t_3 and λ .

Many runs with varying initial estimates of control parameters failed to produce a converged solution. Changes in steam switching times and λ were too severe for the linearizations involved in the quasilinearization algorithm.

6. CONCLUSIONS

- (1) Specification of the control law in a functional form with unknown parameters and optimization of these parameters by a parameter estimation algorithm is shown to be a method of determining sub-optimal control laws for nonlinear systems.
- (2) The technique gives the designer more flexibility than rigorous optimization techniques.
- (3) Numerical instability is encountered in calculating the optimal switching times of a bang-bang type control law unless the initial estimates of these times are near to the optimal values or unless a convergence technique such as constrained parameter perturbation is used. Parameters in smooth functions such as polynomial expansions would be more easily estimated.
- (4) When the form of the optimal control law is known the control policy obtained by this technique can be optimal.

CHAPTER SEVEN

DISCUSSION AND CONCLUSIONS

1. GENERAL DISCUSSION

Quasilinearization and linear programming techniques were applied to optimal state driving control systems. Results in the form of experimental and simulated runs successfully demonstrate the utility of the procedures. Sufficient documentation of runs and computer programs have been provided so that this work could serve as a starting point for future studies or industrial implementation. Documentation includes:

- (1) graphical presentation of runs
- (2) tabular summary of run (simulated and experimental) conditions and parameters
(Appendix C)
- (3) an experimental run book (bound separately)
- (4) documentation of computer programs and example solutions (bound separately from thesis).

In subsequent sections the utility, future work, related problems and overall conclusions of the thesis are presented briefly.

2. INDUSTRIAL USE

The results of the implementation of optimal control strategies on a pilot plant sized evaporation unit indicate the approach used in this work has practical significance. Several features of the control scheme discussed and evaluated in previous chapters are oriented towards industrial implementation and some are summarized in the following sub-sections.

2.1 Generalized Modelling Techniques

Utilization of a generalized parameter estimation algorithm such as the one developed in this work for identification of a process model does not require a thorough knowledge of the numerical methods utilized. The user must simply code his particular process model in FORTRAN and numerically encode the experimental data and system parameters and constraints. Incorporation of a great deal of a priori information into the problem solution in the form of constraints, weighting factors and model features is possible with the algorithm presented.

2.2 Convenient Mathematical Analysis

Linear programming, a familiar mathematical tool in the process industry, is employed in the dynamic optimization of the open-loop process model response. Mathematical analysis using the open-loop model is less complex than that of the closed-loop model. Several popular linear criteria, such as time optimal, sum of absolute errors and minimum rise time, can be used. With convenient addition of constraints on the control and/or state variables the control engineer can tailor the process response.

2.3 Manual Implementations

Open-loop manual implementation of some simple control strategies is practical. Through the use of constraints the control engineer may "ease" into optimal control by limiting magnitudes and rates of process variable changes.

2.4 Addition to DDC System

The optimal control policy based on the open-loop model is added to the existing DDC regulatory feedback control scheme in such a manner that modelling errors and disturbances are compensated for by feedback action. The control scheme automatically reverts to the original DDC regulatory control scheme when the new steady state is reached. Simple FORTRAN programs accomplish this control strategy easily.

3. APPLICATION TO OTHER PROBLEMS

In previous chapters quasilinearization and linear programming were applied to problems arising in the design of a state driving control system. However, many of the advantages of these numerical methods could be exploited in other applications.

3.1 Linear Programming

Mathematical programming techniques are used in many and varied applications. A few applications relevant to this work are worthy of mention.

3.1.1 Curve Fitting

Although linear programming is not frequently used in multiple linear regressions several advantages accrue when it is utilized. The use of linear programming for this statistical task is not new [1-3]. Clare [4] employed this technique to fit a thermodynamic equation of state to PVT data.

Poor data can seriously affect the fit when the Chebyshev criterion is used. But, careful analysis of the solution allows location of gross errors.

Applications closely related to this work are evident:

(a) z transforms

An assumed sampled data model (equation (1)) is to be fitted to a time series of experimental data, $y(k)$ and $u(k)$:

$$\frac{y(z)}{u(z)} = \frac{z^{-i} (a_0 + a_1 z^{-1} + \dots + a_n z^{-n})}{(1 + b_1 z^{-1} + \dots + b_n z^{-n})} \quad (1)$$

In equation (1) i represents a transport delay of i sample times. The problem is to estimate parameters $(a_0, a_1 \dots a_n)$, (b_1, b_2, \dots, b_n) and i . A one dimensional search is required to determine the transport delay. Parameters (a_0, a_1, \dots, a_n) and (b_1, b_2, \dots, b_n) can be evaluated by linear programming. If equation (1) is transformed back to the time domain, the following difference equation is obtained:

$$y_k + \sum_{j=1}^n a_j y_{k-j} = \sum_{j=0}^n a_j u_{k-j-i} \quad (2)$$

$$k = 1, 2, \dots, N$$

The least squares criteria is commonly used to estimate the parameters (Chapter 2, Section 4). If the Chebyshev or the SAE criterion is used, the estimation can be readily formulated in such a manner that linear programming can be utilized.

(b) Laplace transforms

A common problem in control applications is the estimation of parameters in a Laplace transfer function model so as to fit experimental frequency response data. The model is the ratio of two polynomials times a transport delay term:

$$G(s) = \frac{e^{-\tau ds}(a_0 + a_1 s + \dots + a_n s^n)}{(1 + b_1 s + b_2 s^2 + \dots + b_n s^n)} \quad (3)$$

Again the transport delay must be determined by a one dimensional search. To fit the frequency response data s is replaced by $j\omega$ and equation (3) separated into real and imaginary parts:

$$G(j\omega) = \operatorname{Re}(j\omega) + j \operatorname{Im}(j\omega) \quad (4)$$

Least squares techniques are often employed (Chapter 2, Section 7). The criteria used with linear programming must be a linear function of the weighted real deviations and the weighted imaginary deviations.

The advantages of using linear programming over least squares are threefold:

- (1) alleviation of the inherent ill-conditioned phenomenon
- (2) convenient addition of constraints on parameters to force a physically meaningful solution
- (3) convenient constraints on model response to force, for example, known slopes on a Bode plot.

3.1.2 Design of Digital Controllers

An analysis similar to that of section 3.1.1a is applicable to the design of digitally compensated control systems. In this instance (a_0, a_1, \dots, a_n) and (b_1, b_2, \dots, b_n) of equations (1) and (2) are known process parameters and the object is to synthesize a digital controller to make a stable, realizable control system. The digital controller will be assumed to have the following form:

$$D(z) = \frac{(c_0 + c_1 z^{-1} + \dots + c_n z^{-n})}{(1 + d_1 z^{-1} + \dots + d_n z^{-n})} \quad (5)$$

where it remains to determine the constants (c_0, c_1, \dots, c_n) and (d_1, d_2, \dots, d_n). The objective function for the linear programming formulation is the choice of the designer; eg. sum of the absolute sampled errors. The use of linear programming allows constraints on the manipulated variable as well as the sampled errors [5,6].

3.2 Quasilinearization and Linear Programming

The algorithm developed in this work for estimation of parameters in an assumed process model (Chapter 3) or for characterizing an input (Chapter 6) is applicable to many problems which arise in a chemical engineering environment. For example, the algorithm is directly applicable to the two point boundary value problem which arises in optimal control theory from the Pontryagin's Maximum Principle [7]. Application to the adjustment of dynamic process data is a direct extension to the approach used in this work for adjustment of steady state data.

3.2.1 Adjustment of Transient Process Data

A data acquisition and adjustment program was used in this work to obtain a consistent estimate of the stationary state of the plant. Linear programming was utilized in the

adjustment phase of the algorithm. The steady state material and energy balance equations served as linear constraint equations. For the analogous dynamic situation quasilinearization is suitable for generating linear material and energy balance constraint equations.

The adjustment can be performed at each sampling instant assuming input variables constant over the sampling interval (TPBVP). Or the complete set of transient data can be employed (MPBVP) and coefficients in functional approximations to input variables be estimated. The latter would result in smooth curves over the trajectory.

Unknown parameters such as heat transfer coefficients can be estimated along with the state vector. This procedure is for all practical purposes an off-line technique of data adjustment. Kalman filtering techniques [8] are more readily adapted to on-line applications when a control computer is available.

4. FUTURE WORK

Further work with the techniques presented in previous chapters is required in the form of more varied applications, improvements in computational efficiency and implementation, and comparisons with other techniques. The following sub-sections outline the suggestions as applied to the various stages of the optimal state driving design procedure.

4.1 Data Adjustment

(1) The object of the MEBOL program utilized in this work was to obtain a working algorithm which provided a consistent set of data. Hypothesis testing was used in the detection of gross errors and linear programming in the data adjustment. Maximum likelihood estimation is more attractive from a statistical viewpoint. Also it has been suggested that model discrimination procedures on the basis of likelihood ratios would provide an alternate method for detection of gross errors [10]. The technique involves comparing the likelihood ratios of models (ie. steady state material and energy balances) formed by assigning the errors of closure of the balances to each measurement in turn.

(2) The Kalman filter requires estimates of the initial state of the plant and the covariance matrix of the state vector. These can be readily supplied by MEBOL providing an excellent starter for the filter.

4.2 Process Identification

(1) Computational streamlining for the algorithm presented in Chapter 3, was discussed in section 3 of that chapter. The integration phase of the solution warrants the greatest amount of attention. Evaluation of the stability of simplified numerical integration methods at least in phase I of the solution is suggested. Hybrid com-

putation is clearly advantageous.

(2) Comparison of the method described in this work to other procedures on the basis of computational ease, convergence, flexibility and ease of utility is desirable to fully evaluate the power of this approach.

(3) Although the quasilinearization plus linear programming method was applied to several real engineering problems, application to other systems would provide a more complete insight into the advantages of the approach used in this work.

4.3 Dynamic Optimization

(1) Performance of other techniques for computation of optimal controls should be compared to the numerical methods used in this work. Incorporation of constraints on state and control variables, ease of use, and limitations should be considered as well as computational time.

(2) Extension of the linear programming formulation to the approximate solution of continuous linear optimal control problems is easily performed [9].

4.4 Implementation

(1) Although the evaporator used in this work involves unobserved state variables, nonlinearities, control and state constraints and moderate dimensions, implementation of optimal control policies on other processes (such as the

distillation column in the Department of Chemical and Petroleum Engineering at the University of Alberta) would further demonstrate the practicality of the approach.

(2) The concept of using a series of optimal control policies based on linear process models is promising. The process is driven to a pre-arranged state whereupon a new model comes into effect. However the process may or may not attain this desired condition. The feedback implementation introduced in Chapter Six would be useful in this context. An alternative is the use of a nonlinear model.

(3) On-line tuning of switching parameters has obvious advantages. This may be possible only for elementary control laws such as the time optimal control policy based on a single input system described by a second order differential equation.

(4) Control programs used in this work were process programs however they were not incorporated into the DDC monitor system. Development of implementation routines as an integral part of the monitor system would result in more efficient and convenient utility.

5. CONCLUSIONS

Specific conclusions are included in each chapter; however several overall points are evident:

(1) An adjustment program, MEBOL, was developed and used routinely as part of the evaporator run procedure since it provided a consistent set of data for use in subsequent optimization or engineering calculations [11].

(2) Quasilinearization and linear programming combine to make a general and effective parameter estimation algorithm.

(3) The accuracy of a process model is much more critical in state driving control than in regulatory applications. The adequacy of the model must be judged by its performance in actual applications and not by a measure such as the "goodness-of-fit" based on a comparison of the open-loop model responses with experimental data.

(4) Fitted models in general performed better than purely theoretical models in optimal control implementation. Reduced models fitted to the process response resulted in simple control laws which could be tuned experimentally. However, the design procedure for these reduced models did not handle state constraints.

(5) Optimal state driving techniques produce improved performance over conventional three mode control for set-point changes. The advantage of these techniques is particularly evident during large changes such as those that occur during startup.

(6) A control configuration was developed whereby the feedback control loops are not opened during setpoint changes and in fact are used to partially compensate for model inaccuracies and load disturbances. The use of the open-loop model simplified computation. The optimal policy was added to the feedback scheme so that the process automatically reverts to the original regulatory control scheme when the new setpoints are reached.

(7) For certain criteria the optimal control problem for nonlinear systems can be formulated as a parameter estimation problem.

(8) The programs and procedures have been tested on pilot plant equipment and they are considered practical for industrial use. Optimal control policies may be introduced progressively and may incorporate existing procedures.

NOMENCLATURE FOR CHAPTER THREE

<u>A</u>	coefficient matrix
<u>B</u>	basis matrix
<u>b</u>	right-hand-side vector
<u>c</u>	cost vector in LP sense
<u>C</u>	covariance matrix
<u>f</u>	vector of functions in state variable notation
<u>g</u>	vector of functions in augmented state variable notation
<u>J</u>	Jacobian matrix
m	number of inputs
n	number of state variables
N	integer number of data points/sets
p	number of parameters
<u>P</u>	unknown parameters vector
r	number of outputs
s	standard deviation
t	time
<u>u</u>	vector of inputs
<u>v</u>	particular solution
<u>V</u>	variance matrix
w	weighting factor
<u>w</u>	noise vector
<u>x</u>	state vector
<u>y</u>	output vector

Nomenclature for Chapter Three (continued)

z augmented state vector

Z objective function

Subscripts

i state variable subscript

j data set number

k time point number

B basis

DS data sets

p particular

Superscripts

m iteration number

Greek Symbols

ϕ fundamental matrix

ϵ_1 positive deviation

ϵ_2 negative deviation

ω dual variables

λ maximum deviation

NOMENCLATURE FOR CHAPTER FOUR

<u>A</u>	state variable coefficient matrix
<u>B</u>	control variable coefficient matrix
<u>B</u> ₁	first effect bottoms flow rate (lb/min)
<u>B</u> ₂	second effect bottoms flow rate (lb/min)
<u>C</u> ₁	glycol concentration in first effect (wt fraction)
<u>C</u> ₂	glycol concentration in second effect (wt fraction)
<u>C</u> _F	glycol concentration in feed (wt fraction)
<u>e</u> _i	state variable weighting vector at i th sampling instant
<u>F</u>	feed flow rate (lb/min)
<u>K</u> _P	process gain, product concentration to steam
<u>K</u> _L	linear gain, product concentration to steam
<u>O</u> ₁	overhead first effect (lb/min)
<u>O</u> ₂	overhead second effect (lb/min)
<u>P</u> ₁	pressure in first effect vapor space (psig)
<u>r</u>	desired setpoint for y
<u>r</u> ₀	initial setpoint for y
<u>S</u>	steam flow rate (lb/min)
<u>T</u>	sampling time
<u>T</u> ₁	first effect temperature (°F)
<u>T</u> _F	temperature of the feed (°F)
<u>t</u> ₁	switching time equation (5)

Nomenclature for Chapter Four (continued)

t_2	switching time equation (6)
\underline{u}	control variables vector ($m \times 1$)
w_1	first effect liquid holdup (lb)
w_2	second effect liquid holdup (lb)
x	state variables vector ($n \times 1$)
\underline{x}_d	desired state variables vector ($n \times 1$)
\underline{x}_0	initial state variables vector ($n \times 1$)
x'	perturbation variable (x -steady state value)
y	output variable
Δ	control variables coefficient matrix in state difference equation $= \int_0^T \exp(\Delta t) dt \cdot \underline{B} \underline{u}(k)$
λ	maximum deviation
τ_1	major time constant (min)
τ_2	minor time constant (min)
τ_d	time delay (min)
ϕ	fundamental matrix ($e^{\Delta T}$)

NOMENCLATURE FOR CHAPTER FIVE

<u>A</u>	state variable coefficient matrix
<u>B</u>	control variable coefficient matrix
<u>B</u> ₁	bottoms flow from first effect
<u>B</u> ₂	bottoms flow from second effect
<u>C</u> ₂	product concentration
<u>J</u>	performance index
<u>K</u> _p	process gain
<u>m</u>	number of control variables
<u>n</u>	number of state variables
<u>N</u>	total number of sampling instants
<u>S</u>	steam flow rate
<u>s</u>	Laplace transform variable
<u>t</u>	time
<u>u</u>	control vector
<u>w</u> ₁	first effect holdup
<u>w</u> ₂	second effect holdup
<u>x</u>	state vector
<u>Z</u>	objective function in LP formulation
<u>Φ</u>	state variable coefficient matrix in state difference equation
<u>Δ</u>	control vector matrix in state difference equation
<u>τ</u>	time constant

NOMENCLATURE FOR CHAPTER SIX

J index of performance

N number of sampling instants

t time

x state vector ($n \times 1$)

u control vector ($m \times 1$)

λ maximum deviation

Subscripts

o initial

f final

kth sampling instant

d desired

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APPENDIX A

EQUIPMENT DESCRIPTION

A schematic diagram of the evaporator is shown in Figure 1. The unit operates at a throughput of approximately five pounds per minute of three percent aqueous triethylene glycol and produces a product of about ten percent glycol. The first effect is a calendria type unit with an eight inch diameter tube bundle. The second effect is a long tube vertical unit with three one inch by five foot tubes and is operated with forced recirculation. The second effect is operated under vacuum and utilizes the vapor from the first effect as a heating medium.

The evaporator has conventional electronic instrumentation for about fourteen control loops and the recording of over thirty temperatures. In-line refractometers are used for the continuous measurement of feed and product concentrations. All transmitters and final control elements are connected to an IBM 1800 computer. A direct digital control (DDC) monitor system has the capability of implementing conventional three mode control as well as other controller configurations. The digital computer, which operates in a time sharing mode, permits 24 hr/day unattended operation of the evaporator. It also has the capability of data storage, reduction and plotting required in computer control studies such as this work.

The control loops of concern in this work are the loops which control the product concentration and the liquid levels. As represented in Figure 1 these loops are cascaded control loops. Normally the level loops utilize conventional proportional plus integral control with constants which produce "averaging" liquid level control. The product concentration is only run in a closed loop configuration for short periods of time due to refractometer drift. The in-line refractometer which monitors the product concentration must be periodically cleaned. Accurate calibration and temperature compensation is essential.

Implementation of optimal control techniques was facilitated by the fact that the DDC monitor system has provisions for a bias sum which proved to be convenient for addition of open-loop optimal control action:

$$\begin{aligned}\text{Control action} &= \text{proportional} + \text{integral} \\ &\quad + \text{derivative} + \text{bias}\end{aligned}$$

It was necessary to sum the slave loops associated with the bottom flow rates and the steam since rapid manipulated variable response was required in this work.

For equipment details refer to Chapter Four, references [1] and [2].

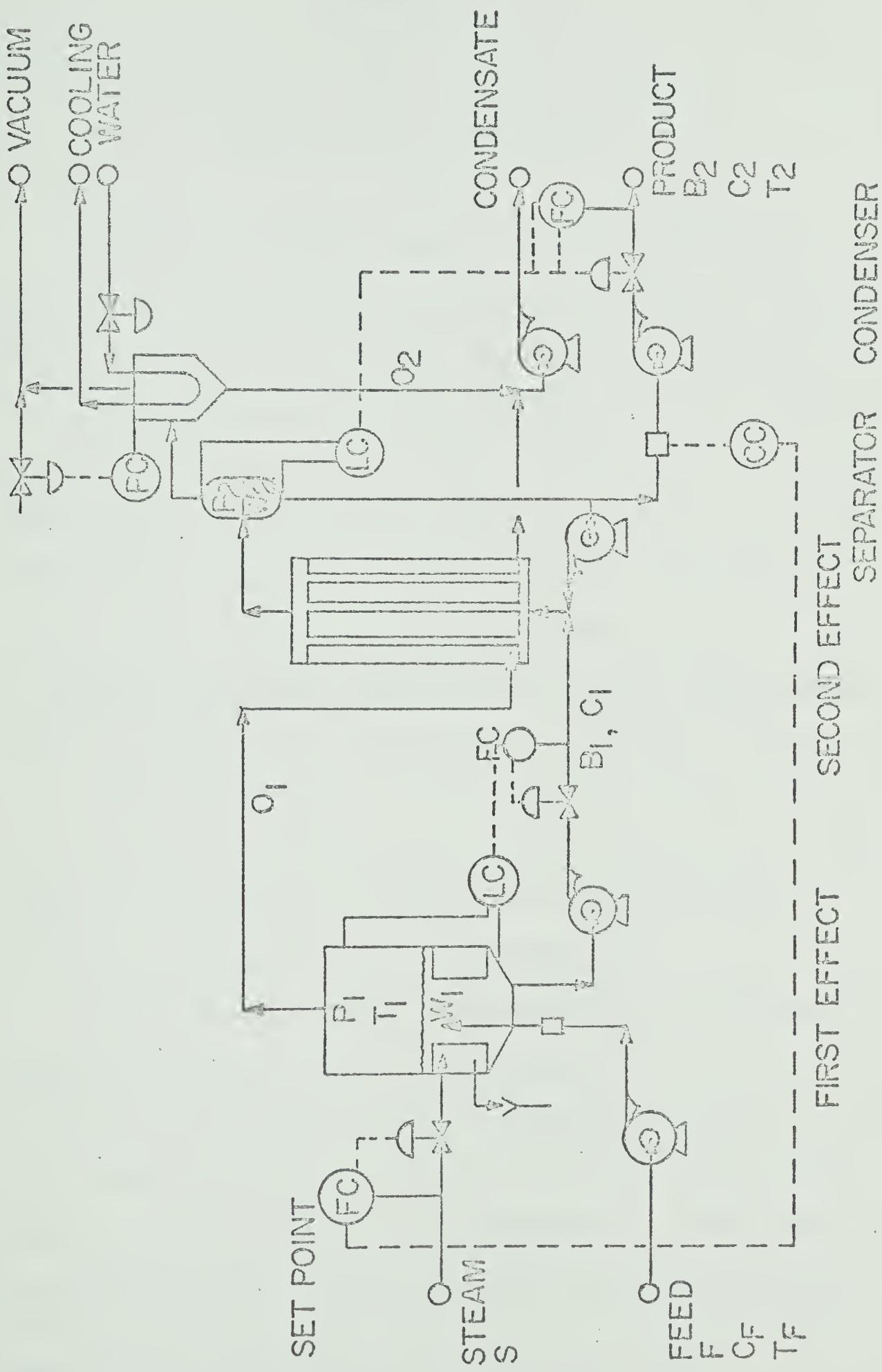


FIGURE 7: Schematic Diagrams of Double Effect Evaporator

APPENDIX B

DOCUMENTATION OF MODELS OF THE
DOUBLE EFFECT EVAPORATOR

The double effect evaporation unit described in Appendix A was modelled for control purposes. This Appendix documents the results of the modelling and identification.

Under the assumption of perfect mixing in both effects and of negligible response time in tube walls and vapor space, material and energy balances result in six first order differential equations. However, since the pressure in the second effect is controlled, the second effect temperature is constant and the second effect energy balance can be used to algebraically evaluate the overhead product flow rate. The remaining five differential equations are listed below along with associated algebraic equations. The complete derivation is presented elsewhere* and is therefore omitted from this presentation.

Reference is made to the nomenclature section of Appendix B and to Figure 1, Appendix A. Tables 1, 2 and 3 list nominal steady states and model parameters. Model 5NL refers to the five equation nonlinear model with theoretical estimates of the parameters. Model 5NLF is the corresponding fitted version (see Chapter Three).

*See Chapter Three References [24] and [25].

Summary of Nonlinear Evaporator Model:

First Effect

$$\text{Mass Balance} \quad \frac{dw_1}{dt} = F - O_1 - B_1$$

$$\text{Component Balance} \quad \frac{dc_1 w_1}{dt} = F c_F - B_1 c_1$$

$$\text{Heat Balance} \quad \frac{dw_1 h_1}{dt} = F h_F + Q_1 - O_1 h_{O_1} - B_1 h_1 - H L_1$$

$$\text{Steam Chest} \quad Q_1 = UA_1(T_c - T_1) = S(h_S - h_c)$$

Second Effect

$$\text{Mass Balance} \quad \frac{dw_2}{dt} = B_1 - O_2 - B_2$$

$$\text{Component Balance} \quad \frac{dc_2 w_2}{dt} = B_1 c_1 - B_2 c_2$$

$$\begin{aligned} \text{Heat Balance} \quad O_2 &= [Q_2 - H L_3 + B_1 \{ (h_1 - h_2) \\ &\quad + \frac{\partial h_2}{\partial c_2} (c_2 - c_1) \}] / [h_{O_2} - h_2 + \frac{\partial h_2}{\partial c_2} c_2] \end{aligned}$$

$$\text{Steam Chest} \quad Q_2 = UA_2(T_1 - T_2) = O_1 (h_{O_1} - h c_L) - H L_2$$

$$\text{Enthalpies} \quad H = 1066.0 + 0.4 T$$

$$h = T(1 - 0.16c) - 32$$

TABLE 1

NOMINAL STEADY STATES

	STEADY STATE 1			STEADY STATE 2		
	Feed	Bottoms 1	Bottoms 2	Steam	Feed	Bottoms 1
Flow rate lb/min)	5.02	3.30	1.66	2.00	5.02	3.16
Concentra- tion (%wt)	3.20	4.85	9.65	0.00	3.2	5.07
Temperature (F)	195.0	227.0	156.3	318.1	195.0	232.9

TABLE 2
MODEL PARAMETERS

MODEL	W1	W2	SS**	HL3/ HL2	UA1	UA2
1	5NL	30.0	35.0	1	3.0	67.0
2	5NLF*	64.7	35.0	1	1.7	67.0
3	5L1	25.0	28.0	1	3.0	23.7
4	5L	30.0	35.0	1	3.0	67.0
5	5LF*	64.7	35.0	1	1.7	67.0
6	5LD	30.0	35.0	2	3.0	23.7

* see Table 3 for details of estimation

** see Table 1

TABLE 3
ESTIMATION OF MODEL PARAMETERS
OF NONLINEAR MODEL
(see Chapter Three)

PARAMETERS	INITIAL ESTIMATE	CONSTRAINTS		FINAL VALUE
		UPPER	LOWER	
UA1	67.0	67.0	67.0	67.0
UA2	23.0	24.0	20.0	23.7
HL1	58.0	48.0	58.0	58.0
HL2	47.0	-----	-----	108.0
HL3	20.0	-----	-----	183.0
W1	30.0	100.	30.	64.7
W2	35.0	100.	35.	35.0

* $HL2 + HL3 =$ heat loss for second effect at $t = 0$.

The nonlinear model was linearized to produce four linear models. Tables 1 and 2 indicate the point of linearization and model parameters used.

A FORTRAN program, LINZD, was written to evaluate the partial derivatives required to obtain the coefficients in the linear model. The program listing is documented and bound separately from the thesis.

The following matrix differential equations are the linearized evaporator models used in this work. The variables in these vector differential equations are perturbation variables (i.e. deviation from nominal steady state, see Tables 1 and 2).

$$\begin{bmatrix} \dot{w}_1 \\ \dot{c}_1 \\ \dot{T}_1 \\ \cdot \\ \dot{w}_2 \\ \cdot \\ \dot{c}_2 \end{bmatrix} = \begin{bmatrix} 0.0 & 0.0 & -0.0243 & 0.0 & 0.0 \\ 0.0 & -0.143 & 0.000051 & 0.0 & 0.0 \\ 0.0 & 0.553 & -1.285 & 0.0 & 0.0 \\ 0.0 & 0.037 & -0.256 & 0.0 & 0.0 \\ 0.0 & 0.118 & 0.000088 & 0.0 & -0.0607 \end{bmatrix} \begin{bmatrix} w_1 \\ c_1 \\ T_1 \\ \cdot \\ w_2 \\ \cdot \\ c_2 \end{bmatrix}$$

$$+ \begin{bmatrix} 0.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 41.75 & 0.0 & 0.0 \\ 0.0 & 0.930 & -1.0 \\ 0.0 & -0.00147 & 0.0 \end{bmatrix} \begin{bmatrix} S \\ B_1 \\ B_2 \end{bmatrix}$$

$$+ \begin{bmatrix} 1.0 & 0.0 & 0.0 \\ -0.000717 & 0.2174 & 0.0 \\ -1.395 & 1.122 & 0.218 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix} \begin{bmatrix} F \\ C_F \\ T_F \end{bmatrix}$$

MODEL 5L1

$$\begin{bmatrix} \dot{w}_1 \\ \dot{c}_1 \\ \dot{T}_1 \\ \dot{w}_2 \\ \dot{c}_2 \end{bmatrix} = \begin{bmatrix} 0.0 & 0.0 & -0.0243 & 0.0 & 0.0 \\ 0.0 & -0.11 & 0.0000 & 0.0 & 0.0 \\ 0.0 & 0.4238 & -0.9850 & 0.0 & 0.0 \\ 0.0 & 0.0372 & -0.0256 & 0.0 & 0.0 \\ 0.0 & 0.0942 & -0.0000 & 0.0 & -0.0485 \end{bmatrix} \begin{bmatrix} w_1 \\ c_1 \\ T_1 \\ w_2 \\ c_2 \end{bmatrix}$$

$$+ \begin{bmatrix} 0.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 32.007 & 0.0 & 0.0 \\ 0.0 & 0.930 & -1.0 \\ 0.0 & -0.00118 & 0.0 \end{bmatrix} \begin{bmatrix} s \\ B_1 \\ B_2 \end{bmatrix}$$

$$+ \begin{bmatrix} 1.0 & 0.0 & 0.0 \\ -0.000549 & 0.1667 & 0.0 \\ -1.0695 & 0.860 & 0.167 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix} \begin{bmatrix} F \\ C_F \\ T_F \end{bmatrix}$$

MODEL 5L

$$\begin{bmatrix} \dot{w}_1 \\ \dot{c}_1 \\ \dot{T}_1 \\ \dot{w}_2 \\ \dot{c}_2 \end{bmatrix} = \begin{bmatrix} 0.0 & 0.0 & -0.025 & 0.0 & 0.0 \\ 0.0 & -0.105 & 0.000 & 0.0 & 0.0 \\ 0.0 & 0.544 & -0.993 & 0.0 & 0.0 \\ 0.0 & 0.039 & -0.025 & 0.0 & 0.0 \\ 0.0 & 0.090 & 0.000 & 0.0 & -0.040 \end{bmatrix} \begin{bmatrix} w_1 \\ c_1 \\ T_1 \\ w_2 \\ c_2 \end{bmatrix}$$

$$+ \begin{bmatrix} 0.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 32.209 & 0.0 & 0.0 \\ 0.0 & 0.924 & -1.0 \\ 0.0 & -0.00163 & 0.0 \end{bmatrix} \begin{bmatrix} s \\ b_1 \\ b_2 \end{bmatrix}$$

$$+ \begin{bmatrix} 1.0 & 0.0 & 0.0 \\ -0.000623 & 0.167 & 0.0 \\ -1.2671 & 1.0189 & 0.1672 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix} \begin{bmatrix} f \\ c_f \\ t_f \end{bmatrix}$$

MODEL 5LD

$$\begin{bmatrix} \dot{w}_1 \\ \dot{c}_1 \\ \dot{T}_1 \\ \dot{w}_2 \\ \dot{c}_2 \end{bmatrix} = \begin{bmatrix} 0.0 & 0.0 & -0.0237 & 0.0 & 0.0 \\ 0.0 & -0.051 & 0.0000 & 0.0 & 0.0 \\ 0.0 & 0.197 & -0.4472 & 0.0 & 0.0 \\ 0.0 & 0.0372 & -0.02493 & 0.0 & 0.0 \\ 0.0 & 0.0941 & 0.0000 & 0.0 & -0.04562 \end{bmatrix} \begin{bmatrix} w_1 \\ c_1 \\ T_1 \\ w_2 \\ c_2 \end{bmatrix}$$

$$+ \begin{bmatrix} 0.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 14.841 & 0.0 & 0.0 \\ 0.0 & 0.9301 & -1.0 \\ 0.0 & -0.0012 & 0.0 \end{bmatrix} \begin{bmatrix} s \\ B_1 \\ B_2 \end{bmatrix}$$

$$+ \begin{bmatrix} 1.0 & 0.0 & 0.0 \\ -0.000255 & 0.0773 & 0.0 \\ -0.4959 & 0.39877 & 0.07749 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix} \begin{bmatrix} F \\ C_F \\ T_F \end{bmatrix}$$

MODEL 5LF

Nomenclature for Appendix B

B	bottom flow rate (lb/min)
C	concentration (wt. percent)
F	feed rate (lb/min)
h	liquid enthalpy (Btu/lb)
H	vapor enthalpy (Btu/lb)
HL ₁	heat loss first effect (Btu/min)
HL ₂	heat loss second effect steam chest (Btu/min)
HL ₃	heat loss second effect solution (Btu/min)
O	overhead rate (lb/min)
Q	heat transfer (Btu/min)
S	steam rate (lb/min)
T	temperature (°F)
UA	overall heat transfer coefficient times area (Btu/min°F)
W	holdup (lb)

Subscripts

1	first effect
2	second effect
F	feed
0	overhead
c	condensate

APPENDIX C

Run Documentation

The following Tables summarize the data necessary to duplicate the experimental and/or simulated runs presented in the preceding chapters. This data is meant to supplement the Figures in which they are used, therefore data available from the Figures is not reproduced. A complete compilation of all run data including material and energy balance data is on file with the Department of Chemical and Petroleum Engineering. Errors of closure were usually less than five percent.

In many of the simulations and experimental runs a control policy is derived from one model and implemented on a more rigorous model or on the process. This Table identifies models (Appendix B), documents state variable weighting, state and control constraints and other data relevant to the simulation, dynamic optimization or experimental run.

The abbreviations used in the Tables are defined at the end of the Appendix. The run numbers are those which appear in the run book. The Figure numbers are those of the previous chapters in which the response is plotted.

The actual listings of programs, input data and computer output for many simulations are included in user documentation which was bound separately.

TABLE 1

EXPERIMENTAL RUNS

RUN	FIG.	CONTROL MODEL (5)			PROCESS (6)			COMMENTS			
		MODEL	CONSTRAINTS STATE		IP	WEIGHT	F	CF	LLC	CC	
OSD3	4-3	order 1 (1)			T.O.	C ₂ only	4.5	3.0	tight P		unable to close C loop (t _f) refractometer poor
OSD6	4-6	order 2 (2)	1.0 ≤ S ≤ 2.4								
OSD7	4-6	order 3 (3)									
OSD12	4-10	5L ₁	1.0 ≤ S ≤ 3.58	T ₁ ≤ 13°	T.O.	C ₂ , W ₁	5.0	3.0	OL		refractometer poor manipulated variable response poor
OSD13	4-11	5L ₁	0 ≤ B ₁ ≤ 6.24 0 ≤ B ₂ ≤ 2.66	-5.0 ≤ W ₁ ≤ 5.0 -5.0 ≤ W ₂ ≤ 5.0		C ₂ , W ₂					
						C ₂ only					
JC16	4-5	order 1	1.0 ≤ S ≤ 2.3		T.O.	C ₂ only	4.5	3.0	tight P	PP	noisy B ₂ affected refractometer
JC17	4-4	order 1									
JC20	4-8	order 2 (4)	1.0 ≤ S ≤ 2.2		T.O.	C ₂ only	4.5	3.0	tight P	PP	
JC21	4-9	order 2									
JC22	4-5, 8										
JC23	4-4, 9										
JC14	4-5, 8										
JC15	4-4, 9										
JC28	lost data	order 2 (7)	1.0 ≤ S ≤ 2.2		T.O.	C ₂ only	4.5	3.0	tight P	FB(8)	poor model (up)
JC30	not used	order 2 (7)	1.0 ≤ S ≤ 2.2								
JC31	5-12	order 2 (7)	1.0 ≤ S ≤ 2.2		T.O.	C ₂ only	4.5	3.0	tight OL	FB(8)	poor model (down)
JC29	5-12	order 2 (7)	1.0 ≤ S ≤ 2.2								

(1) Refer to Chapter Three (2) Refer to Table 1, Chapter Four (model 3) (4) $\tau_1 = 1.85$, $\tau_2 = 44$ (adapted by trial and error using OPTIM)
 (5) All runs on this page 16 sec. Sampling interval (6) $T_F = 1900F$ for all runs

TABLE I (cont'd)

RUN	FIG	CONTROL MODEL (5)			PROCESS (6)			COMMENTS			
		MODEL	CONSTRAINTS	STATE	IP	WEIGHT	F	C_F	LLC	CC	
JC32a	5-6	order 2	(4) 1. $0 \leq S \leq 2.2$	T.0	C_2 only	$\frac{4.5}{4.5}$	3.0 tight	$\frac{0L}{FB}(8)$			good 2nd order empir- ical control model
JC32b	5-16	order 2	(4) 1. $0 \leq S \leq 2.2$	T.0	C_2 only	$\frac{4.5-4.0}{4.5-4.0}$	3.0 tight	$\frac{0L}{FB}(8)$			feed dis- turbance
JC33	5-15	order 2	(4) 1. $0 \leq S \leq 2.2$	T.0	C_2 only	$\frac{4.5-4.0}{4.5-4.0}$	3.0 tight	$\frac{0L}{FB}(8)$			feed dis- turbance
JC37	5-13	order 2	(4) 1. $0 \leq S \leq 2.2$	T.0	C_2 only	$\frac{4.5-5.0}{4.5-5.0}$	3.0 tight	$\frac{0L}{FB}(8)$			feed dis- turbance
JC34	5-16	order 2	(4) 1. $0 \leq S \leq 2.2$	T.0	C_2 only	$\frac{4.5-5.0}{4.5-5.0}$	3.0 tight	$\frac{0L}{FB}(8)$			feed dis- turbance
JC36	5-16	order 2	(4) 1. $0 \leq S \leq 2.2$	T.0	C_2 only	$\frac{4.5-5.0}{4.5-5.0}$	3.0 tight	$\frac{0L}{FB}(8)$			feed dis- turbance
JC38	5-6	5L	1. $0 \leq S \leq 3.0$ 0. $0 \leq B_1 \leq 62.8$ 0. $0 \leq B_2 \leq 2.66$	T.0	C_2 only	5.0	3.0 0L	0L			
JC39	5-7	5LF	"	"	T.0	C_2 only	5.0	3.0 0L	0L		
JC40	5-8	5LF	"	"	"	"	"	"	"		
JC42	5-10	5LF	"	"	SAE	$\frac{W_1 C_1}{W_2 C_2}(S)$	3.2	"	"		
JC43	5-18	5LF	"	"	SAE	"	"	EB(7) $\frac{FB}{FB}(7)$			no output lim- it so steam valve blew
JC44	5-18	5LF	"	"	SAE	"	"	"	"		output limit
JC45a	5-19	5LF	"	"	"	"	"	"	"		
JC45c	5-19	5LF	"	"	"	"	"	"	0L	0L	

(7) $T_1 (k_P = 20^\circ\text{F}) T_2 (g) 25 (\dot{m}_0, 1, T_0 = 0^\circ\text{F}, T = 32 \text{ sec.}$ (8) Feed back of the type depicted in Figure

TABLE 2
SIMULATIONS

SIMULA-TION	FIGS	MODEL	CONTROL MODEL			PROCESS MODEL					
			CONSTRAINTS	STATE	IP	WEIGHTS	MODEL	F	C _F	LLC	CC
1	4-2,6	order (1)	$1.0 \leq S \leq 2.5$	T.O.	C_2 only		5NL	4.5	3.0	tight P	0L
2	4-2	order 2								avg P+I	DDC setpoint change
3	4-2									avg P+I	0L
4	4-3	order (2)	$1.0 \leq S \leq 2.5$	T.O.	C_2 only		5NL	4.5	3.0	tight P	0L
5		order (1)								avg P+I	0L
6	4-7	order (2)	$1.0 \leq S \leq 2.5$	T.O.	C_2 only		5NL	4.5	3.0	tight P	RT
7	4-10	5L1	$1.0 \leq S \leq 3.58$ $0.0 \leq B_1 \leq 6.24$ $0.0 \leq B_2 \leq 2.66$	P ₁ ≤ 10 psig -5.0 ≤ W_1 ≤ 5.0 -5.0 ≤ W_2 ≤ 5.0	T.O.	C_2, W_1, W_2 C_2 only	5NL	5.0	3.0	0L	0L
8	4-11										
9	6-1	5NL	$1.0 \leq S \leq 3.0$	P ₁ ≤ 10 psig C_2 overshoot	MRT	C_2 only	5NL	5.0	3.0	tight P	0L
10	6-1	5NL		P ₁ ≤ 10 psig C_2	MRT	C_2 only	5NL	5.0	3.2	tight P	P+I
11	5-6	5L	$1.0 \leq S \leq 3.0$ $0 \leq B_1 \leq 6.24$ $0 \leq B_2 \leq 5.0$	T ₁ ≤ 13.0 -5.0 ≤ W_1 ≤ 5.0 -5.0 ≤ W_2 ≤ 5.0	T.O.	C_2 only	5L	5.0	3.02	0L	0L

(1) See Table 1, Chapter 4; (2) See Chapter 4; (3) (10 1 1 10 100) using normalized perturbation variables
 (4) Table 5-1; (5) FB of Figure 5-4; (6) Refer to Chapter Five, equations (10) and (11); (7) X_6 limits on over and undershoot at all sampling points ($\sim \frac{1}{4}$ damping) ($\pm 5\% T_S$) ($X_1 - X_5$) - limits at all sampling points, see simulation output for details.

TABLE 2 (cont'd)

SIMULATION	FIGS	CONTROL MODEL						PROCESS MODEL					
		MODEL		CONSTRAINTS		IP		WEIGHTS		MODEL		C	
		CONTROL	STATE	same	same	T.O.	C_2 only	5NL	5.0	3.02	0L	C_F	CC
12	5-9	5L	same	same	same	T.O.	C_2 only	5NL	5.0	3.02	0L	0L	
13	5-9	5LD	same	same	same	T.O.	C_2 only						
14	5-10	5LF (4)	same	same	same	SAE Note(3)		5LF	5.0	3.02	0L	0L	
15	5-11	order 2 (4)	$1.0 \leq S \leq 2.2$			T.O.	C_2 only	5NL	5.0	3.02	tight P	$\frac{0L}{FB(5)}$	
16	5-11	order 2 (4)	$1.0 \leq S \leq 2.2$			T.O.	C_2 only	5NL	5.0	3.02	tight P	$\frac{0L}{FB(5)}$	
17	5-13	order 2 (4)	$1.0 \leq S \leq 2.2$			T.O.	C_2 only	5NL	5.0	3.02	tight P	$\frac{0L}{FB(5)}$	
18	5-13	order 2 (4)	$1.0 \leq S \leq 2.2$			T.O.	C_2 only	5NL	5.0	3.02	tight P	$\frac{0L}{FB(5)}$	
19	5-14	order 2 (4)	$1.0 \leq S \leq 2.2$			T.O.	C_2 only	5NL	4.5-5.0	3.02	tight P	$\frac{0L}{FB(5)}$	
20	5-14	order 2 (4)	$1.0 \leq S \leq 2.2$			T.O.	C_2 only	5NL	4.5-5.0	3.02	tight P	$\frac{0L}{FB(5)}$	
21	5-16	order 2 (4)	$1.0 \leq S \leq 2.2$			T.O.	C_2 only	5NL	4.5-5.0	3.02	tight P	$\frac{0L}{FB(5)}$	
22	5-16	absorber (6) (linear)	$0.0 \leq u_1 \leq 1.0$ $0.0 \leq u_2 \leq 1.0$			T.O.	equal	absolu-					
23	4-2,3	absorber (6) (linear)	$0.0 \leq u_1 \leq 1.0$ $0.0 \leq u_2 \leq 1.0$			all (7)	MRT	x_5 only (linear)					
24	4-2,3					SAE	unequal (8)						
25	4-2,3											0L	some constraints violated

Abbreviations used in Tables 1 and 2

P	proportional
OL	open loop
PP	phase plane switching
P + I	proportional plus integral control
tight	tight setpoint control
avg	averaging control
T.O.	time optimal
FB	feedback compensation
SAE	sum of absolute errors
LLC	liquid level control law
CC	concentration control law
IP	objective function
F	feedrate
c_F	feed concentration
RT	real time switching
MRT	minimum rise time
T_S	settle outime

APPENDICES FOR CHAPTER THREE

Appendix 1

Derivation of Nonlinear Gain Expression

The nonlinear gain expression can be derived directly from the nonlinear model. Assuming a stationary state exists, the differential equations of Appendix B become algebraic equations. In subsequent equations variables will be represented as X and $X + \Delta X$ where X represents the initial state and ΔX the offset produced from a perturbation in an input variable. The input perturbation considered here will be a change in steam flow rate, ΔS . From the energy balance around the first effect steam chest (Appendix B)

$$Q_1 = S(H_S - h_c) \quad (1)$$

and T_F are assumed to be constant throughout.

From first effect mass balance:

$$\Delta B_1 = -\Delta O_1 \quad (2)$$

Assuming T_F is the saturation temperature and neglecting the effect of small concentration and temperature changes on enthalpy:

$$\Delta S(H_S - h_c) - \Delta B_1 h_1 - \Delta O_1 H_{O_1} = 0 \quad (3)$$

$$\text{or } \Delta Q_1 = \left(\frac{H_S - h_c}{H_{O_1} - h_1} \right) \Delta S \quad (4)$$

$$= k_1 \Delta S \quad (5)$$

From the energy balance around the second effect steam chest

$$\Delta Q_2 = \Delta Q_1 H_{V_1} \quad (6)$$

where H_{V_1} is the latent heat of vaporization for water at temperature T_1 .

Considering the component balance around the first effect:

$$C_1 + \Delta C_1 = \frac{F c_F}{B_1 + \Delta B_1} \quad (7)$$

$$\text{or } \Delta C_1 = \frac{-C_1 \Delta B_1}{(B_1 + \Delta B_1)} \quad (8)$$

$$\Delta C_1 = \frac{C_1 k_1 \Delta S}{B_1 - k_1 \Delta S} \quad (9)$$

From the mass balance around the second effect:

$$\Delta B_2 = \Delta B_1 - \Delta Q_2 \quad (10)$$

From the component balance around the second effect:

$$\Delta C_2 = \frac{B_1 \Delta C_1 + \Delta B_1 (C_1 + \Delta C_1) - \Delta B_2 C_2}{B_2 + \Delta B_2} \quad (11)$$

or substituting for ΔB_1 using equations (2) and (5) and simplifying:

$$\Delta C_2 = \frac{k_1 (C_2 + k_2 C_2) \Delta S}{B_2 - k_1 (1 + k_2) \Delta S} \quad (12)$$

where

$$k_2 = \frac{H_{V_1} - (T_1 - T_2)}{H_{V_2}} \quad (13)$$

Evaluating the linearized equivalent to (9) and (12)
ie.:

$$K_{L_1} = \left. \frac{\partial}{\partial S} \left(\frac{C_1 k_1 \Delta S}{B_1 + k_1 \Delta S} \right) \right|_{\Delta S=0}$$

$$K_{L_1} = \frac{k_1 C_1}{B_1} \quad (14)$$

$$\text{similarly } K_{L_2} = \frac{k_1 (1 + k_2) C_2}{B_2} \quad (15)$$

Substituting (14) and (15) into (9) and (13):

$$\frac{\Delta C_1}{\Delta S} = \frac{K_{L_1}}{1 - K_{L_1} \Delta S / C_1} \quad (16)$$

$$\frac{\Delta C_2}{\Delta S} = \frac{K_{L_2}}{1 - K_{L_2} \frac{\Delta S/C_2}{C_2}} \quad (17)$$

$$\frac{\Delta C_2}{\Delta S} = K_{L_2} \left(1 + \frac{\Delta C_2}{C_2} \right) \quad (18)$$

Equation (17) is useful in predicting the gain for open-loop simulations of the process to step changes in steam rate. However, in the servomechanism problem when the change in C_2 is known, ΔC_2 , a more useful form of the gain equation is equation (18).

Figure 1 indicates the performance obtained from this nonlinear gain expression. Experimental data for the steady state gain are very scattered when raw data is used. Adjusted values of the product concentration, the symbols in Figure 1, yield better results.

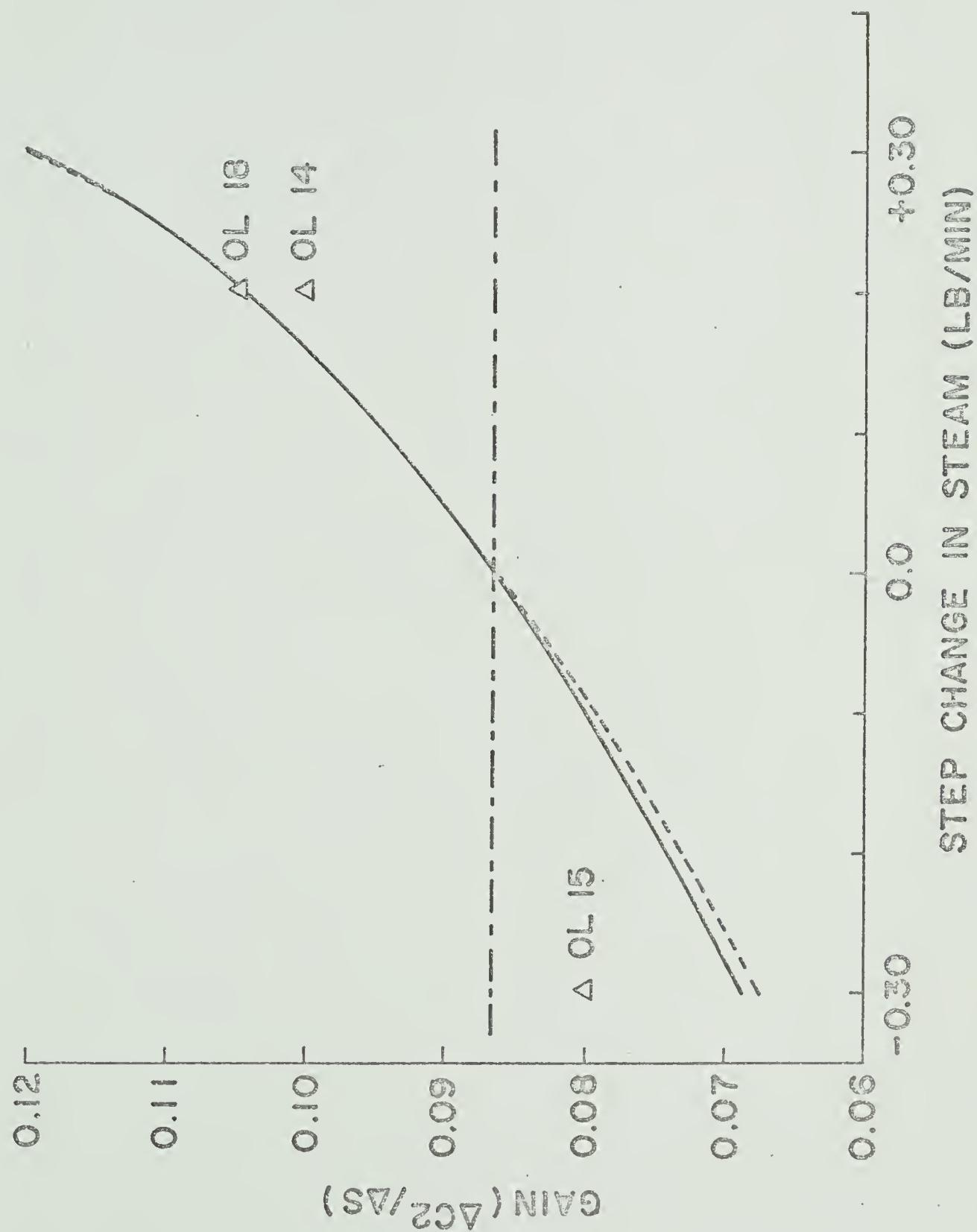


FIGURE 1: Comparison of Steady State Gain
 - - - 5L, — 5NL, --- gain expression,
 Δ experimental.

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